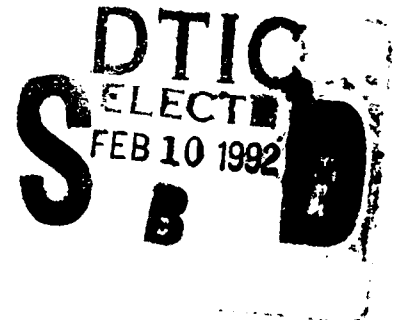


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THESIS

CLUSTER MODEL OF
POLARIZATION UPON REFLECTION
FROM METALLIC SURFACES

by

Craig Wesley Baldwin

December, 1991

Thesis Advisor:

Oscar Biblarz

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19 ABSTRACT (continue on reverse if necessary and identify by block number) POLARIZATION OF LIGHT IS AT BEST ONLY PARTIALLY EXPLAINED BY CURRENT MODELS. A NEW MODEL IS PROPOSED TO ACCOUNT FOR THIS PHENOMENON INVOLVING "NATIVE CLUSTERS". THESE CLUSTERS ARE ASSUMED TO BE AN INTEGRAL PART OF SOME BULK SURFACES AND TO MANIFEST THEIR DIELECTRIC PROPERTIES IN THE VISIBLE REGION. AN INDEX OF REFRACTION MAY BE COMPUTED BASED ON A PSEUDO-BREWSTER ANGLE, THAT ANGLE OF INCIDENCE WHERE THE MINIMUM PERPENDICULAR REFLECTANCE OCCURS. NEXT THE MODEL IDENTIFIES THE CLUSTER-TO-BULK SURFACE AREA RATIO OF THE MATERIAL AND FORMULATES THE CONTRIBUTION OF REFLECTION FROM THESE AREAS BY UTILIZING THE FRESNEL EQUATIONS. REFLECTANCE FROM THE REMAINDER, THE BULK SURFACE AREA, IS COMPUTED BY APPLYING CONVENTIONAL METALLIC REFLECTION TECHNIQUES. BY COMBINING THE TWO CONTRIBUTIONS OF REFLECTANCE FOR ANGLES OF INCIDENCE FROM 0 TO 90 DEGREES, REFLECTANCE CURVES ARE GENERATED FOR GOLD, SILVER, NICKEL AND ALUMINUM. THESE CALCULATIONS ASSUME A WIDE-BAND RADIATING SOURCE OF LIGHT. ALTHOUGH THE MAGNITUDE OF REFLECTANCE FOR THE MODEL SHOWED SOME VARIANCE OVER THE RANGE OF ANGLES OF INCIDENCE (1 WITHIN 10%), THE CURVES ARE SIMILAR IN SHAPE. THE MINIMUM PERPENDICULAR REFLECTANCE AND GRAZING ANGLES OF INCIDENCE ARE CONSISTENT WITH EXPERIMENTAL FINDINGS. THE COMPUTED SURFACE RATIO FOR EACH METAL VARIES INDIRECTLY WITH THE METAL'S NORMAL REFLECTANCE VALUE, AS EXPECTED FROM THE MODEL. SPECTRAL INFORMATION ON THE COMPLEX INDEX OF REFRACTION IS INCLUDED TO INFER PROBABLE CLUSTER SIZE.				
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Cluster Model of
Polarization Upon Reflection
From Metallic Surfaces

by

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Lieutenant Commander, United States Navy
B.S., Purdue University 1979

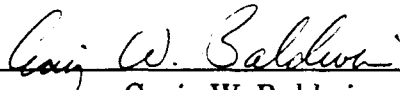
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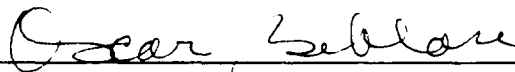
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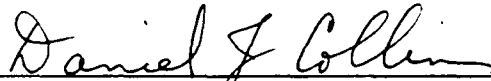

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ABSTRACT

Polarization of light due to metallic reflection is at best only partially explained by current models. A new model is proposed to account for this phenomenon involving "native clusters". These clusters are assumed to be an integral part of metallic bulk surfaces and to manifest their dielectric properties in the visible region. An index of refraction may be computed based on a pseudo-Brewster angle, that angle of incidence where the minimum perpendicular reflectance occurs. Next the model identifies the cluster-to-bulk surface area ratio of the material and formulates the contribution of reflection from these areas by utilizing the Fresnel equations. Reflectance from the remainder, the bulk-surface area, is computed by applying conventional metallic reflection techniques. By combining the two contributions of reflectance for angles of incidence from 0 to 90 degrees, reflectance curves are generated for gold, silver, nickel and aluminum. These calculations assume a wide-band radiating source of light. Although the magnitude of reflectance for the model showed some variance over the range of angles of incidence (within 10%), the curves are similar in shape. The minimum perpendicular reflectance and grazing angles of incidence are consistent with experimental findings. The computed surface ratio for each metal varies indirectly with the metals' normal reflectance value, as expected from the model. Spectral information on the complex index of refraction is included to infer probable cluster size.



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I. DESCRIPTION OF MECHANISMS FOR METALLIC REFLECTION

A. INTRODUCTION

Optical polarization was discovered by E. L. Malus in 1808. However, it was not until the nineteenth century and the formulation of electromagnetic theory developed by Maxwell that this phenomenon could be described analytically, at least partially. Moreover, the theory addresses the results more than the mechanism. J. Bennett and E. Bennett from the Naval Weapons Center are quoted in Ref. 1 as saying in reference to the electromagnetic theory,

"This theory is phenomenological in that instead of trying to explain why materials have certain fundamental characteristics, it concentrates on the resulting properties which any material with those characteristics will display. Electromagnetic theory has little or nothing to say about why a material should have these particular optical properties ..."

This is a strong statement concerning the present lack of understanding involved in the polarization process during metallic reflection. Bennett and Bennett continue to state that at the present time solid state physics can only partially explain the mechanism which causes polarization for some surfaces. In this chapter, currently accepted mechanisms are mentioned and the concept of "native clusters" will be introduced.

B. PRESENT SCOPE OF RESEARCH

Clusters are a collection of atoms which have properties between bulk and molecular entities. Clusters are also known as microparticles, or finite systems. They

are primarily studied in the free state [Ref. 2]. "Native clusters" [Ref. 3], refer to the covalent aggregation of a fixed number of atoms at the surface energy level of the metal. This clustering is presumed to exist at all times, although the cluster site position on the surface, varies with time.

Having performed a thorough literature search, and having been sponsored by the Naval Postgraduate school to attend an international symposium on the physics and chemistry of finite systems [Ref 4], the author has found that presently there is intense interest within the scientific community concerning clusters. However, despite the wide-ranging topic material presented at the conference [Ref. 4], there is a noticeable lack of research involving bound "native clusters" and their impact on surface science. It appears that the main thrust at present, is on defining, building and manipulating the free clusters, which are created through vaporization of bulk material by high energy lasers. Since, as stated in Refs. 2 & 4, free clusters are derived from the bulk material and by themselves display properties other than the bulk from which they were produced and that many clusters assembled together begin to take on the properties of the bulk, it seems logical that research involving "native clusters" would add to the understanding of how clusters, a distinct phase of matter [Ref 2], interact within metallic surfaces and modify their emission behavior.

C. MECHANISMS OF POLARIZATION

Currently there are two accepted models which partially describe the behavior of reflected waves from metallic surfaces: The free electron theory which is best suited for

the infrared spectrum and below and, conversely the quantum model works well in the ultraviolet region of the energy spectrum and beyond.

1. Free Electron Theory

The free electron theory is based on a model where actually, two types of electrons reside on the surface. Bound electrons or electrons which are covalently bonded to the atoms which make up the crystalline surface of the metal and free electrons which are associated with good conductors and are free to move about in a random pattern thereby producing no net current [Ref. 5]. Introducing the complex index of refraction, the interaction of the free electrons with an electromagnetic wave can be accounted for by the imaginary part, which in turn depends on the properties of the metal. More specifically, on the conductivity as it relates to the number of free electrons in the metal [Ref. 5]. However, as one will note in Chapter III, the model is limited to the portion of the spectrum in the infrared (IR). However, two important facts are validated by this model.

- Electromagnetic waves in the near infrared and longer wavelengths are exclusively absorbed at the surface by interaction with the free electrons. (see Chapter III)
- Magnitudes of parallel and perpendicular polarized reflectance can be obtained from the Fresnel equations over the same portion of the energy spectrum given above.

2. Quantum Mechanics

For reasons explained in Chapter III the quantum model is best suited for explaining the mechanism in the ultraviolet (UV) and higher energy portion of the spectrum. High energy waves possess enough energy to influence conduction bands, it

is theorized, above the Fermi level but below the work function level. If this is the case then it may be possible to associate these bands with dipoles which are the necessary ingredient for polarization to occur. However, this linkage is not well developed at this time due to the complexity of the interaction between high frequency waves and the band electrons [Ref. 5].

3. Polarization Due To "Native Clusters"

"Native clusters" are postulated to exist as discrete sites on the surface, to be transparent and non-absorbing in the visible portion of the spectrum [Ref. 6]. The theory that "native clusters" do exist on metallic surfaces is proposed in Ref. 3. In this work, Bibiarz complements the free electron model used in describing thermionic emission from metals. It is postulated [Ref. 3], that clusters are intrinsic regions which exist on the surface of bulk metal and which alter all emission properties of the bulk (i.e., electron, atom and photonic). A thermionic model is developed which includes "native clusters" as a percentage of the total surface area of the metal. Combining the bulk contribution to the contribution from the clusters, the total thermionic emission is determined over a range of temperatures. As shown in Ref. 3, this model better predicts thermionic emission than the pure free electron model in the case of refractory metals.

The conjectured shape of clusters is interesting from the standpoint of their integration into the bulk surface. Clusters are mostly surface area. In fact Ref. 2 states that tightly packed clusters of 20 atoms may have only one atom in their interior. This would lead one to think of clusters as having much more surface than depth when composing a portion of the bulk metal. Further hampering the defining of the cluster

shape is the inability to observe cluster atomic structure directly with current electron microscopy methods if the cluster is less than about two nanometers in size [Ref. 4]. However, some cluster shapes are being inferred from mass spectral data and magic numbers associated with the material [Ref. 4].

If the cluster size is around one micrometer across [Ref. 3], then one can discount from being applicable to this model those portions of the spectrum which are made up of wavelengths either too big to affect the cluster or are so small that their interaction with the electrons in the cluster is negligible. For these portions of the spectrum, either the free electron model for long wavelengths or the quantum model for short wavelengths may be a more satisfactory explanation of the mechanism.

Free metallic clusters can be created through vaporization of the bulk metal by high energy lasers. Clusters created in this manner, when studied, do not have the same optical properties as the bulk [Ref. 2]. Therefore, it is reasonable to assume that clusters residing as a portion of the total metallic surface would not share the host optical properties and, in fact, could have the properties stated at the beginning of this chapter. Hence, it follows that if the clusters do exhibit dielectric behavior, their presence can be accounted for in the theory of electromagnetic radiation and by the Fresnel equations. By adding this portion to the contribution from the bulk (free electrons), total metallic reflectance may thus be determined. As such, a mechanism whereby waves of the near IR and visible portion of the spectrum are polarized, is established.

II. BACKGROUND ON ELECTROMAGNETIC WAVE BEHAVIOR

When an electromagnetic wave encounters a boundary between two different optical media, such as an air-dielectric system, it is well known that the wave is resolved into two component parts, one being the reflected wave the other being the transmitted wave [Ref. 7]. In this work we consider "white" light and unpolarized electromagnetic waves, and as such, several properties of the wave as it encounters a dielectric boundary can be explained by electromagnetic theory based on Maxwell's equations [Ref. 5].

A. INDEX OF REFRACTION

The speed of light in vacuum is defined and given by Equation 2.1 below.

$$c = \frac{1}{\sqrt{\mu_0 \epsilon_0}} \quad (2.1)$$

Where μ_0 is the permeability of free space and ϵ_0 is the permittivity of free space.

For optical materials, the index of refraction is defined to be the ratio between the speed of light (c) in a vacuum and the speed of light in the medium (v) [Ref. 7] and is given below in Equation 2.2.

$$n = \frac{c}{v} \quad (2.2)$$

However, for the derivations that follow it will be more correct to make a substitution for v in Equation 2.2 as follows: It is understood [Ref. 5] that for good dielectrics the magnetic permeability (μ) of the dielectric is equal to the magnetic permeability of free

space. Therefore it follows from electromagnetic theory that the velocity of the wave (light) in the dielectric as given by Equation 2.3 [Ref. 7].

$$v = \frac{1}{\sqrt{\mu_0 \epsilon'}} \quad (2.3)$$

Finally, by substitution of Equations 2.1 and 2.3 into Equation 2.2 the index of refraction for dielectrics is given by Equation 2.4.

$$n = \frac{\sqrt{\mu_0 \epsilon'}}{\sqrt{\mu_0 \epsilon_0}} = \sqrt{\frac{\epsilon'}{\epsilon_0}} \equiv \sqrt{\epsilon} \quad (2.4)$$

For the remainder of this paper the permittivity term (ϵ) will refer to a relative permittivity defined as the ratio of permittivity of the dielectric over permittivity of free space. It should be noted that the index of refraction for dielectrics is a real number unlike the index of refraction for conductors which is given in complex form. The reason for this difference will become clear later.

The index of refraction is useful in defining a relationship between the angle of incidence (ϕ) of the incident wave and the refraction angle (ϕ') of the refracted wave (Figure 2.1) known as Snell's law [Ref. 7].

$$\frac{\sin \phi}{\sin \phi'} = \frac{n'}{n} \quad (2.5)$$

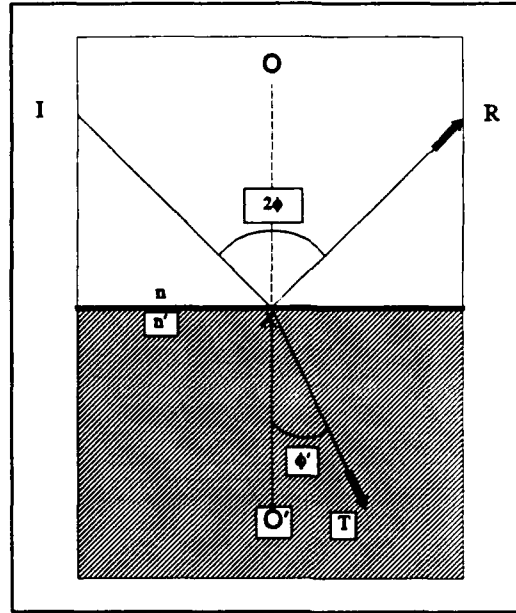


Figure 2.1 Diagram Of Reflection And Refraction Between Two Optical Media n and n'

B. FRESNEL EQUATIONS FOR DIELECTRICS

The description of the Fresnel equations for the transmitted and reflected light waves is straightforward and summarized below. A detailed derivation can be found in any book on electromagnetic wave propagation, such as Ref. 5.

Once a light wave encounters a dielectric boundary, the wave is split into two new waves. From Figure 2.1, one will note there is a reflected wave and a transmitted wave each with a parallel and perpendicular polarization component associated with it. If we let the amplitudes of the incident, reflected, and transmitted waves be denoted by I , R , T , respectively, as shown in Figure 2.1, then apply the boundary condition that the

tangential components be continuous across the boundary [Ref. 8], the results are given by Equation 2.6 [Ref 5].

Since the assumption was made in Ref. 8 that the clusters behave as a dielectric, $n' = \sqrt{\epsilon}$. Making this substitution into the above equation and solving for R_{\perp} , R_{\parallel} , T_{\perp} , T_{\parallel} the well known Fresnel equations for reflectance are obtained and given below by Equation 2.7.

$$\begin{aligned}\cos\phi' T_{\parallel} &= \cos\phi (A_{\parallel} - R_{\parallel}) \\ \sqrt{\epsilon_2} T_{\parallel} &= \sqrt{\epsilon_1} (A_{\parallel} + R_{\parallel}) \\ T_{\perp} &= A_{\perp} + R_{\perp} \\ \sqrt{\epsilon_2} \cos\phi' T_{\perp} &= \sqrt{\epsilon_1} (A_{\perp} + R_{\perp})\end{aligned}\tag{2.6}$$

$$\begin{aligned}RSDP &= \left| \frac{R_{\parallel}}{A_{\parallel}} \right|^2 = \left[\frac{\tan(\phi_i - \phi')}{\tan(\phi_i + \phi')} \right]^2 \\ RSDS &= \left| \frac{R_{\perp}}{A_{\perp}} \right|^2 = \left[\frac{\sin(\phi_i - \phi')}{\sin(\phi_i + \phi')} \right]^2\end{aligned}\tag{2.7}$$

Note that RSDP and RSDS are reflectance coefficients and are the result of squaring the magnitudes of the intensities of the reflected and incident waves, as in evaluation of the pointing vector, then dividing by the square of the component amplitude of the incident wave which normalizes the equations.

C. BREWSTER'S LAW FOR DIELECTRICS

Brewster's law simply states that there exists a specific angle of incidence which is material dependent, such that the reflected light from the dielectric is plane polarized

(i.e., RSDP = 0). From the top formula in Equations 2.7 one will note that this can only occur when the angle between the reflected and transmitted waves is 90° ($\phi_i + \phi' = 90^\circ$) and hence the tangent goes to infinity. The definition of the Brewster angle, leads to Equation 2.8. This angle will be relevant to the development of the "native cluster" model, in Chapter IV.

$$\tan\theta = \frac{n'}{n} \quad (2.8)$$

D. REFLECTION AND REFRACTION PROPERTIES OF A CONDUCTOR

When an electromagnetic wave impinges on a metallic boundary (i.e., a good conductor) a surface current is immediately established . Unlike dielectrics, whose surface structure is composed of bound atoms and electrons, a conductor's surface is usually composed of small non orientated crystals containing free electrons. These free electrons will move so as to cause a surface current when in the presence of an external electric field.

1. Complex Index Of Refraction

According to [Ref. 5], by replacing the real index of refraction (n) as given in Equation 2.4, to a complex index of refraction (N) defined by Equation 2.9 an elementary model can be developed whereby the optical constants ϵ , σ , μ , are utilized as in Equation 2.10, it defines the real and imaginary parts of the complex index of refraction. Note that σ is the conductivity of the metal.

$$N = n - ik \quad (2.9)$$

$$\begin{aligned} n^2 &= \frac{1}{2} \left[\sqrt{\mu^2 \epsilon^2 + \frac{4 \mu^2 \sigma^2}{v^2}} + \mu \epsilon \right] \\ n^2 k^2 &= \frac{1}{2} \left[\sqrt{\mu^2 \epsilon^2 + \frac{4 \mu^2 \sigma^2}{v^2}} - \mu \epsilon \right] \end{aligned} \quad (2.10)$$

Work published in 1903 by E. Haygen and H. Rubens [Ref. 5] indicates that the results of Equations 2.10 are accurate for wavelengths of 10^{-3} cm (infrared waves) or longer. This however, will lead to some error between the calculated and experimental results of these optical properties in the visible to ultraviolet portion of the spectrum. Therefore, this model needs to be restricted to near infrared wavelengths. Notwithstanding the aforementioned, the complex index of refraction arises when dielectric electromagnetic theory is expanded to encompass conductors. Figure 2.2 from Ref. 1, shows the trends in the reflectance curves for increasing n and k . It is particularly helpful in showing that wave propagation into the conductor is small, and hence can be neglected. By defining the "skin-depth" (d) as the distance an electromagnetic wave will travel into a conductor before dissipation of it's energy to a value of $1/e$, and linking this to the inverse of the extinction coefficient [Ref. 5], one can show that the distance of wave propagation into the medium is given by Equation 2.11.

$$d = \frac{c}{\sqrt{8\pi\mu\sigma\omega}} \quad (2.11)$$

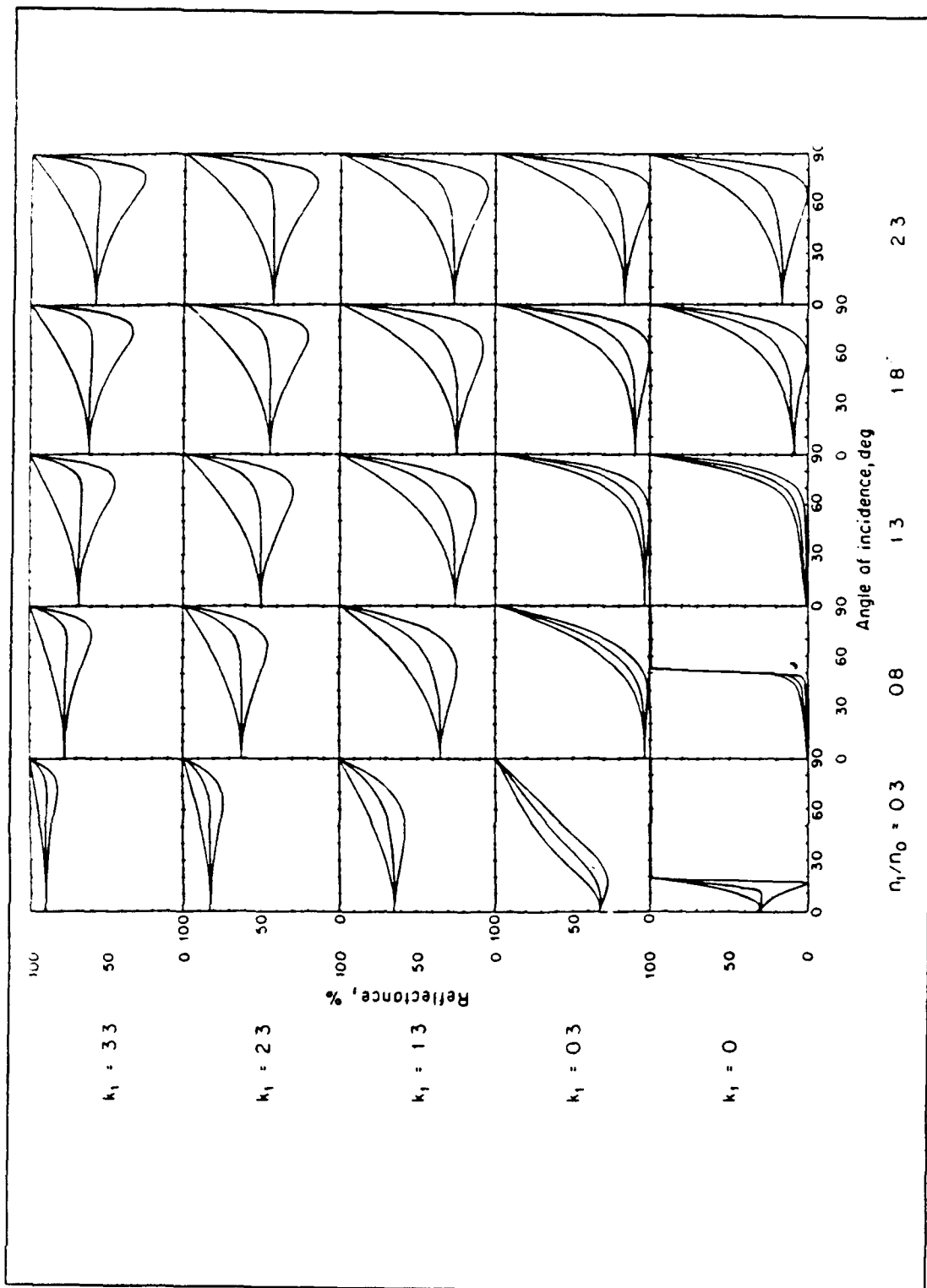


Figure 2.2 Reflectance curves for various values of n and k derived from the free electron model.

From Equation 2.11, one will note that high conductivity (on the order of 10^{17} sec Gaussian units) and high frequencies, as in visible waves, will result in a very small skin depth. As proof an example of how little the wave will be transmitted into the conductor, Ref. 5 gives a skin depth of $d = 10^{-7}$ cm for infrared wave into copper a typical metallic conductor. This fact plays an important role in the development of the bulk reflection model as outlined in Chapter IV, since we can consider the metals to be opaque in the visible portion of the spectrum.

III. FREE ELECTRON AND QUANTUM MODELS

A. THE FREE ELECTRON MODEL OF METALLIC REFLECTION

In Chapter II, wave reflectance from a conductor was addressed using the classical electromagnetic theory based on Maxwell's equations, together with the introduction of the complex index of refraction. In this section the free electron model (proposed by P. Drude) will be shown and comments on its short comings in dealing with the higher frequency wave reflectance will be made.

The basis of the theory for the free electron model is that in a good conductor two types of electrons must reside at the surface. The first type are called bound electrons, or those which are held in a quasi-rigid state by the parent atom, similar to the dielectric. The second type, called free electrons, is a well established model for conductors, in that the surface is full of these electrons which are not bound to any atom and can move fairly freely about. As discussed in the previous chapter, the complex index of refraction is frequency dependent. However, Ref. 5 states that the complex conductivity and emissivity are both frequency dependent, which is shown by Equations 3.4 and 3.6.

1. Derivation Of The Complex Conductivity Term

From statistical methods of the theory of kinetics of gases, the motion of the free electrons can be described by a model of a proportional damping force acting in the opposite direction of the free electron motion [Ref 5]. This motion which is cyclic in nature due to the electric field being cyclic, can be described by the standard second

order differential equation of motion for a damped spring mass system under the influence of the forcing function \vec{E} as shown below.

$$m\ddot{\vec{r}} + m\beta\dot{\vec{r}} = e\vec{E} \quad (3.1)$$

The solution of Equation 3.1 is given in complex form below (i = imaginary index).

$$\vec{r} = -\left[\frac{e}{m(\omega^2 + i\beta\omega)}\right]\vec{E} \quad (3.2)$$

Where \vec{r} is the position vector of the periodic motion of frequency (ω) the electron in an electric field with a damping coefficient (β). The decay time (τ) is inversely related to the damping coefficient (β) which is on the order of 10^{-14} sec [Ref. 5]. Differentiating Equation 3.2, to obtain the velocity of the electron, and substituting this into Equation 3.3 below

$$\vec{J} = N_e e \dot{\vec{r}} = \left[\frac{N_e e^2}{m(\beta - i\omega)}\right]\vec{E} \quad (3.3)$$

and finally using the constitutive relation between current density (\vec{j}) and the electric field (\vec{E}) viz. $\vec{j} = \sigma\vec{E}$ and substituting for σ from Equation 3.3 the result is [Ref. 5]

$$\sigma = \frac{N_e e^2}{m(\beta - i\omega)} \quad (3.4)$$

Note that N_e is the number of free electrons in the conducting band. Thus the dependency on frequency for conductivity is established which will be important in the analysis of the model later in the chapter.

2. Complex Emissivity

As stated in Chapter II for conductors, the index of refraction is complex and since

$$n = \sqrt{\frac{\mu \epsilon'}{\mu_0 \epsilon_0}} = \sqrt{\epsilon} \quad (3.5)$$

It follows that if the index of refraction is complex then, by definition as shown in Equation 3.5, so must the emissivity be complex. For low frequencies Ref. 5 states that the real part of ϵ is small compared to the imaginary part and hence Equation 2.9 becomes the expression for the complex ϵ .

$$\hat{\epsilon} \equiv N^2 = 1 - \left[\frac{4\pi N_e e^2}{m\omega(\omega - i\beta)} \right] \quad (3.6)$$

Hence the dependence on frequency is again established as it was for the conductivity.

3. Analysis Of The Free Electron Model

The free electron model as presented predicts well the optical constants of the conductor for long wavelengths (IR, near or far), but does not accurately predict the behavior of the constants and hence, the reflection of the wave, in the visible portion of the energy spectrum. Evidence of this is presented in Ref. 5. The problem stems from the fact that Equation 3.6 as stated above is derived based on low frequency electric fields, in order to eliminate the contribution of the bound electrons. However, the contribution from the bound electrons becomes more significant as the frequency

increases thereby leading to the breakdown in the model. It is stated in Ref. 5 that the free electron model can not be modified in order to extend it's usefulness into the higher frequency ranges due to the complexity of the interaction between the electric field and the metal in these ranges. It refers the reader to the theory of quantum mechanics for an explanation.

B. QUANTUM THEORY

Band theory of solids is presented in various references (see, for example, Ref. 9). For metals, the theory seems most appropriate in the violet and smaller wavelengths. Interband electron transitions in the near infrared are best known in semiconductors. The quantum mechanical expression for the polarizability is of the same form as that obtained from the classical (Drude) model.

Weak interband transitions appear to decrease the reflectance of aluminum around 1.4 eV . In silver, the reflectance, well into the "vacuum" ultraviolet region, is characteristic of interband transitions spread over a wide spectral region. At 3.9 eV a sharp decrease in reflectance identifies the free-electron plasma frequency. Plasma oscillations are a non-quantum, collective oscillation of the free electrons. Discussion of the present state of this field is beyond the scope of this work.

IV. MODEL DEVELOPMENT

A. "NATIVE CLUSTER" DESCRIPTION

"Native clusters" are postulated to be clusters which form not as a result of the presence of "foreign" atoms deposited on the surface, but rather because of an equilibrium of surface atom configurations [Ref. 3]. The "native cluster" model (Figure 4.1) is able to account for a number of the "nonconductor" properties of reflected light from metallic surfaces since in a cluster, the electrons remain attached to the atoms which make up the cluster and hence do not contribute to the Fermi level. Biblarz postulates in Ref. 6 that a patchwork of "native clusters" that exist on virgin metallic surfaces (based on work published in Ref. 3) does alter polarization upon metallic reflection. The dispersement of such "native clusters" over the bulk surface may produce dispersed dipoles thereby providing the surface with "nonconductor" attributes as exhibited by polarization, by the reflection of visible light from the surfaces, as well as other attributes.

B. FORMULATION OF EQUATIONS

Based on Ref. 3, there is assumed to exist an equilibrium surface area ratio of cluster to bulk material unique to any given metal. Therefore reflected light will have contributions from the bulk (r_B) and clusters (r_S). The total surface area (S_T) is defined as the sum of the cluster area (S_S) and the bulk area (S_B) as shown in Equation 4.1.

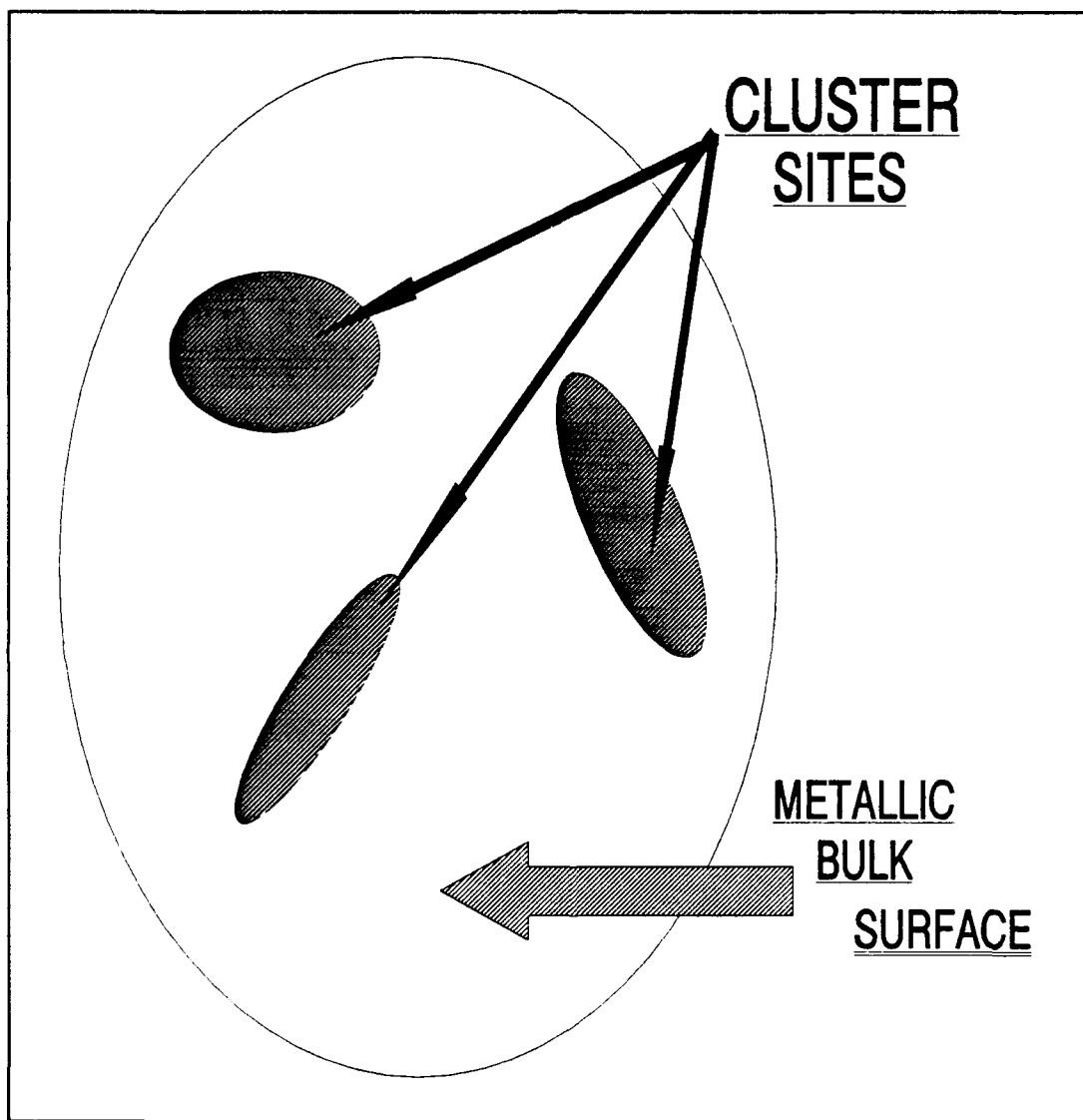


Figure 4.1 Schematic Of Metallic Bulk Cluster Aggregate (Top View)

$$S_S + S_B = S_T \quad (4.1)$$

Dividing Equation 4.1 by the total surface area (normalizing) and defining the fraction S_S/S_T as x , the cluster to total surface ratio, one can substitute this value into Equation 4.1 and solve for the normalized bulk to total surface area ratio as in Equation 4.2.

$$(1 - x) = \frac{S_B}{S_T} \quad (4.2)$$

Total reflectance (r_T) is then given in [Ref. 5] as

$$r_T = (1 - x) r_B + x r_S \quad (4.3)$$

Since the bulk can be considered opaque in the near IR and visible portion of the spectrum [Ref. 6] (the skin depth being on the order of 10^{-7} cm), the contribution from the bulk is simply the reflectance of the bulk times it's normalized surface area. However, clusters behaving as dielectrics, are presumed to be transparent and will allow a portion of the waves to be transmitted through the cluster and then reflected by the metallic substrate while the remainder is reflected directly at the surface. As such, reflectance from the clusters maybe composed of direct reflectance (r_{sd}) and indirect reflectance (r_{si}) leading to

$$r_S = r_{sd} + r_{si} \quad (4.4)$$

A gray body is defined to have characteristics of a black body where the absorptance is equal to the emittance. Assuming that the metallic surface behaves as a gray body (a good assumption for infrared to visible wavelengths) then the absorptance must equal the emissivity (Kirchhoff's law) [Ref. 1] as shown in Equation 4.5.

$$\alpha(\lambda, T) = \epsilon(\lambda, T) \quad (4.5)$$

Energy flux incident on surface can be reflected, transmitted, or absorbed. Applying Equation 4.5 to the flux balance equation [Ref. 1] the relationship between absorptance (α or ϵ), reflectance (r) and transmittance (τ) is shown to be

$$\epsilon(\lambda, \phi, T) + r(\lambda, \phi, T) + \tau(\lambda, \phi, T) = 1 \quad (4.6)$$

C. BULK REFLECTANCE

Transmittance of the light wave into the bulk is shown to be negligible as stated in Ref. 5, hence Equation 4.6 may be written as

$$r_B = 1 - \epsilon(\lambda, T) \cos \phi \quad (4.7)$$

The angle of incidence (ϕ) is defined as the angle between the incident ray and the normal to the surface (see Figure 2.1).

According to Ref. 6 the emittance is well represented in the IR region of the spectrum by Equation 4.8,

$$\epsilon(\lambda, T) = 36.5 \sqrt{\rho(\text{ohm-cm}) / \lambda(\mu\text{m})} \quad (4.8)$$

where ρ (a function of temperature) is the resistivity of the metal in ohm-cm and λ is the wavelength of the incident wave in μm . The non-spectral form of the emittance is determined by integrating over the entire spectrum and shown in Equation 4.9.

$$\epsilon(T) \cong 0.5753 \sqrt{\rho(\text{ohm-cm}) \cdot T_s(K)} \quad (4.9)$$

D. CLUSTER REFLECTANCE

Native clusters possessing dielectric properties will cause incident waves to either be reflected directly (r_{sd}) or indirectly (r_{si}) after transmission through the cluster and reflection from the metallic substrate (see Figure 4.2). As shown by Equation 4.4.

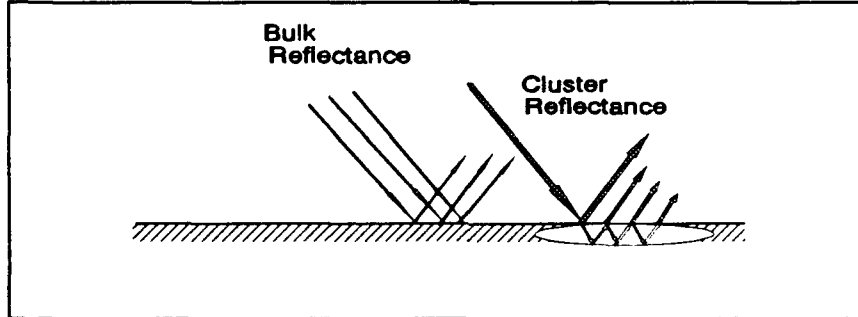


Figure 4.2 Bulk and Cluster Reflection Patterns

1. Direct Cluster Reflectance

Direct cluster reflectance is calculated using the Fresnel equations for dielectrics [Ref. 7]. The reflected light has two components, parallel and perpendicular, representing the polarization effect upon reflection from a dielectric.

2. Indirect Cluster Reflectance

The indirect portion of the reflection is much more difficult to define as it requires knowledge of the shape and size of clusters. Some insight regarding the size of the "native cluster" is discussed in Chapter VI. No attempt was made to include this contribution but preliminary estimates indicate that the magnitude of the contribution to reflection will be on the order of 20% or less.

V. COMPUTER MODEL DESIGN

A. COMPUTER ALGORITHM DEVELOPMENT

Utilizing equations derived in Chapter IV, a computer algorithm named "REFLECTA" (see Appendix A) was developed to calculate the parallel (RTOTLS) and perpendicular (RTOTALP) reflectance from the metallic surface for angles of incidence from 0° to 90° . Reflectance curves were generated from the data by invoking "Easy-Plot", a locally developed software package used with FORTRAN VII at the Naval Postgraduate School, and plotting RTOTLP or RTOTLS against the angle of incidence (ϕ) for each metal.

B. CURVE FITTING

White light reflectance curves for gold, and silver based on experimental results [Ref. 7], were considered to be the baseline from which the "native cluster" model could be compared to, then scrutinized for similarities and differences. Being able to produce reflectance curves from the model which matched the experimental curves, would be proof for the validation of the model.

Three parameters, bulk-cluster index of refraction (n'), cluster to bulk surface area ratio (x) and emittance (ϵ) were utilized in obtaining the best curve fit for a particular metal.

C. EQUATIONS USED IN COMPUTER ANALYSIS

Initially the parameters were fixed, based on results reported in Ref. 7 for gold and silver, which measured reflectance from a "white" tungsten light bulb, probably operating at 3000 K. Plots for these curves are shown in Chapter VI as Figures 6.1 and 6.2. However, curves were also generated for aluminum and nickel in order to expand the data base for future trend analysis (see Figures 6.3 and 6.4). Referring to the REFLECTA program, four terms were considered a critical part in plotting of the reflectance coefficient curves, and are defined below for continuity purposes as they will be repeatedly referred to in the remainder of the thesis.

- RTOTLP is the total surface parallel reflectance coefficient of the metallic surface.
- RTOTLS is the total surface perpendicular reflectance coefficient of the metallic surface.
- RSDP is the parallel reflectance coefficient contribution from direct cluster reflection (Equation 5.1).
- RSDS is the perpendicular reflectance coefficient contribution from direct cluster reflection (Equation 5.2).

RSDS and RSDP were calculated by Equations 5.1 and 5.2.

$$RSDS = \left[\frac{\sin(\phi - \phi')}{\sin(\phi + \phi')} \right]^2 \quad (5.1)$$

$$RSDP = \left[\frac{\tan(\phi - \phi')}{\tan(\phi + \phi')} \right]^2 \quad (5.2)$$

From Equations 5.3 and 5.4, RTOTLP and RTOTLS were calculated.

$$RTOTLS = (1 - x)RB + xRSDS \quad (5.3)$$

$$RTOTLP = (1 - x)RB + xRSDP \quad (5.4)$$

It was noted that the angle of incidence where RTOTLP was a minimum occurred about four degrees right of the experimental curve given in Ref. 7. By noting that this minimum is associated with the pseudo-Brewster angle for the metal, as defined by the minimum perpendicular reflectance as shown in Ref. 7, calculation of the index of refraction for the bulk-cluster aggregate (n') is determined by the following equation.

$$n' = n_1 \tan \phi_{\min} \quad (5.5)$$

where ϕ_{\min} is the pseudo-Brewster angle and n_1 is the index of refraction of air or vacuum (equal to 1.0). However, by adjusting the incident angle to match the experimental pseudo-Brewster angle the entire reflectance curve was shifted up or down depending on the direction of shift in ϕ caused by the matching of the pseudo-Brewster angle. At this point it became clear that a sensitivity analysis for each parameter was required in order to formulate a systematic approach whereby, the three parameters could be varied in a convergent manner thus providing the best curve fit by the model.

D. SENSITIVITY ANALYSIS OF PARAMETERS

As stated above in Section B of this chapter, due to the interdependence of the three parameters used in the generation of the curves and their complexity it is necessary

to perform an analysis on each parameter in order to determine what effect a small change in each has on the reflectance curves.

1. Procedure

Sensitivity testing was performed using gold, by varying one parameter in small increments while holding the other two constant. Total reflectance was recorded at two angles of incidence each chosen for their critical nature in the curve. The first was at $\phi = 2^\circ$ where the incident light is virtually normal and hence the $\cos(\phi)$ is nearly one thereby eliminating the dependence of angle of incidence at that point. The second is located at a point where RTOTLP is at a minimum since, this will provide the best information on curve shifts due to small parameter changes at the Brewster angle. It is felt that the best curve fit would be obtained if these points could be made to match with experimental results.

2. Findings From Sensitivity Analysis

The results of the sensitivity testing are shown in Figure 5.1 and are summarized below.

- Small changes in the parameters produced linear increments of change in the curves.
- Increasing x decreased RTOTLP at $\phi = 2^\circ$ and the minimum RTOTLP. There was no change in ϕ_{\min} , which was expected since this is governed by n' only.
- Varying ϵ had no effect on the shape of the curves. Thus this parameter can be determined by Equation 4.9 and fixed.
- Increasing n' increases RTOTLP at $\phi = 2^\circ$; produces no change in RTOTLP_{min}; and increases ϕ_{\min} .

3. Partial Conclusions From Sensitivity Analysis

From the displayed linearity above and the equation of a line we can generate two simultaneous equations. Letting y be the value of RTOTLP at an angle of incidence equal to 2° , we can solve for the two unknowns, slope of the line (m) and the intercept (b) for a given n' , set initially by the pseudo-Brewster angle. Once this is accomplished, the value for x can be determined for that metal by setting y equal to the experimental value of RTOTLP at normal incidence and solving for x . The curves are then generated using these parameter values. The angle of incidence corresponding to $RTOTLP_{min}$ is compared with the experimental value and a small change is made in n' in order to shift the curve towards the experimental. This new n' is then used in determining a new value for x and the process repeats itself until ϕ_{min} experimental matches with that of the program. It's important to note at this time that the initial estimate of x should be chosen so as to comply with current wisdom regarding the area ratio of cluster to bulk.

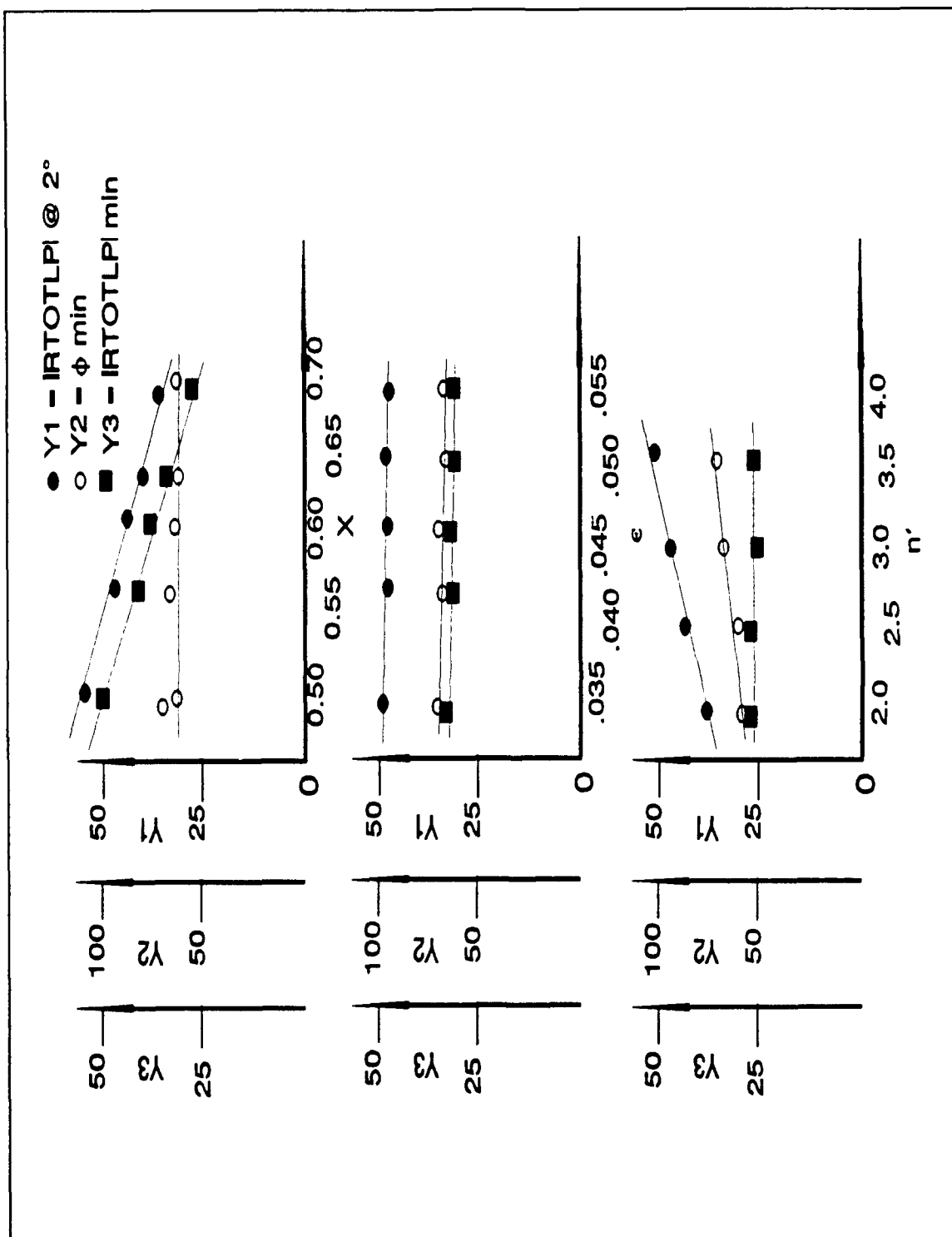


Figure 5.1 Parameter Sensitivity Plots For Gold

VI. RESULTS

A. CURVE FIT EXPERIMENTAL VERSUS THE MODEL

Utilizing the aforementioned "native cluster" model and the computer algorithm developed in the previous chapter, total reflectance curves were generated for four metals, gold, aluminum, nickel, and silver (Figures 6.1 thru 6.4). These data as well the results produced by the model are for wide-band light (i.e., white light) where the source temperature was assumed to be 3000 K. Experimental values for gold and silver are shown as x's. The definition of these parameters is necessary in order to incorporate the experimental curves displayed in Ref. 7, for comparison purposes to those of the model.

Comparison of the reflectance curves produced by the model to the experimental curves given in Ref. 6 reveal the following similarities listed below.

- At normal incidence ($\phi = 0^\circ$), both parallel and perpendicular reflectance have the same magnitudes. Further, this common magnitude is in agreement with the value measured by experimental means.
- Perpendicular reflectance increases as the angle of incidence increases throughout the range of values in a similar fashion to the experimental values.
- Parallel reflectance decreases to a minimum located at an angle of incidence associated with the pseudo Brewster angle of the metal as does the experimental value of parallel reflectance.
- Parallel reflectance increases for angles of incidence greater than the pseudo-Brewster angle to the grazing angle of incidence ($\phi = 90^\circ$).

TOTAL REFLECTANCE (GOLD)

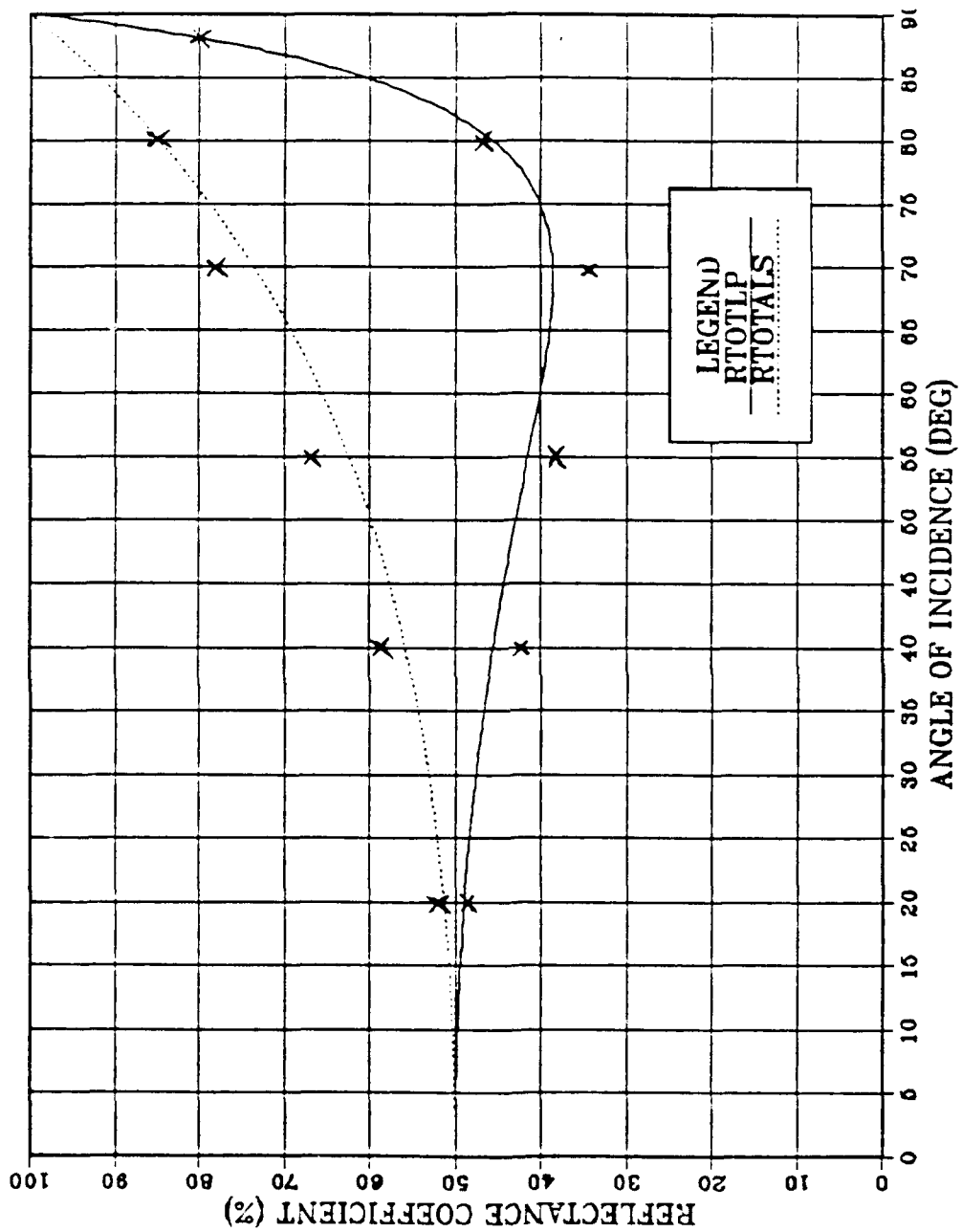


Figure 6.1 Reflectance Curves Of Gold. x's correspond to measurements from Ref. 7.

TOTAL REFLECTANCE (SILVER)

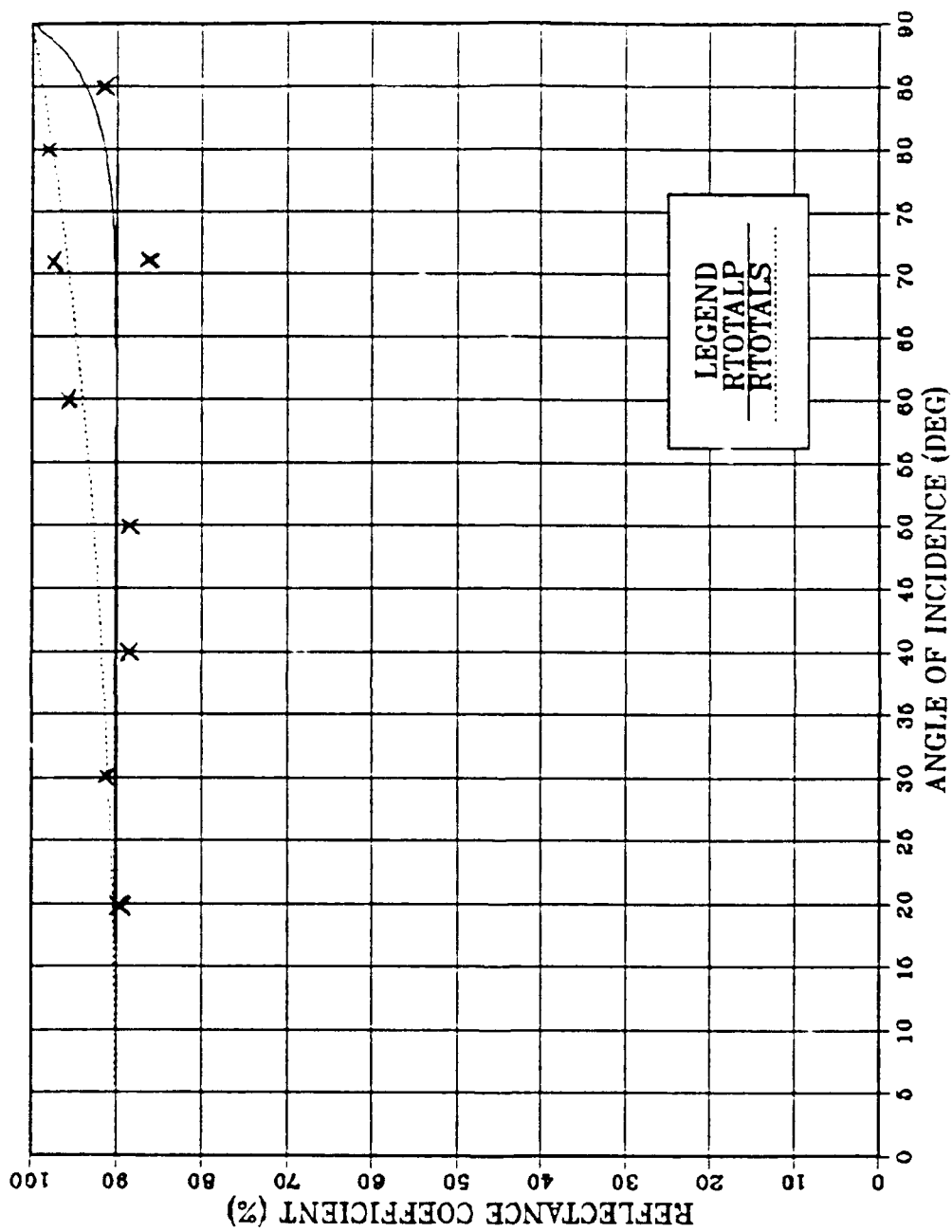


Figure 6.2 Reflectance Curves Of Silver. x's correspond to measurements from Ref. 7.

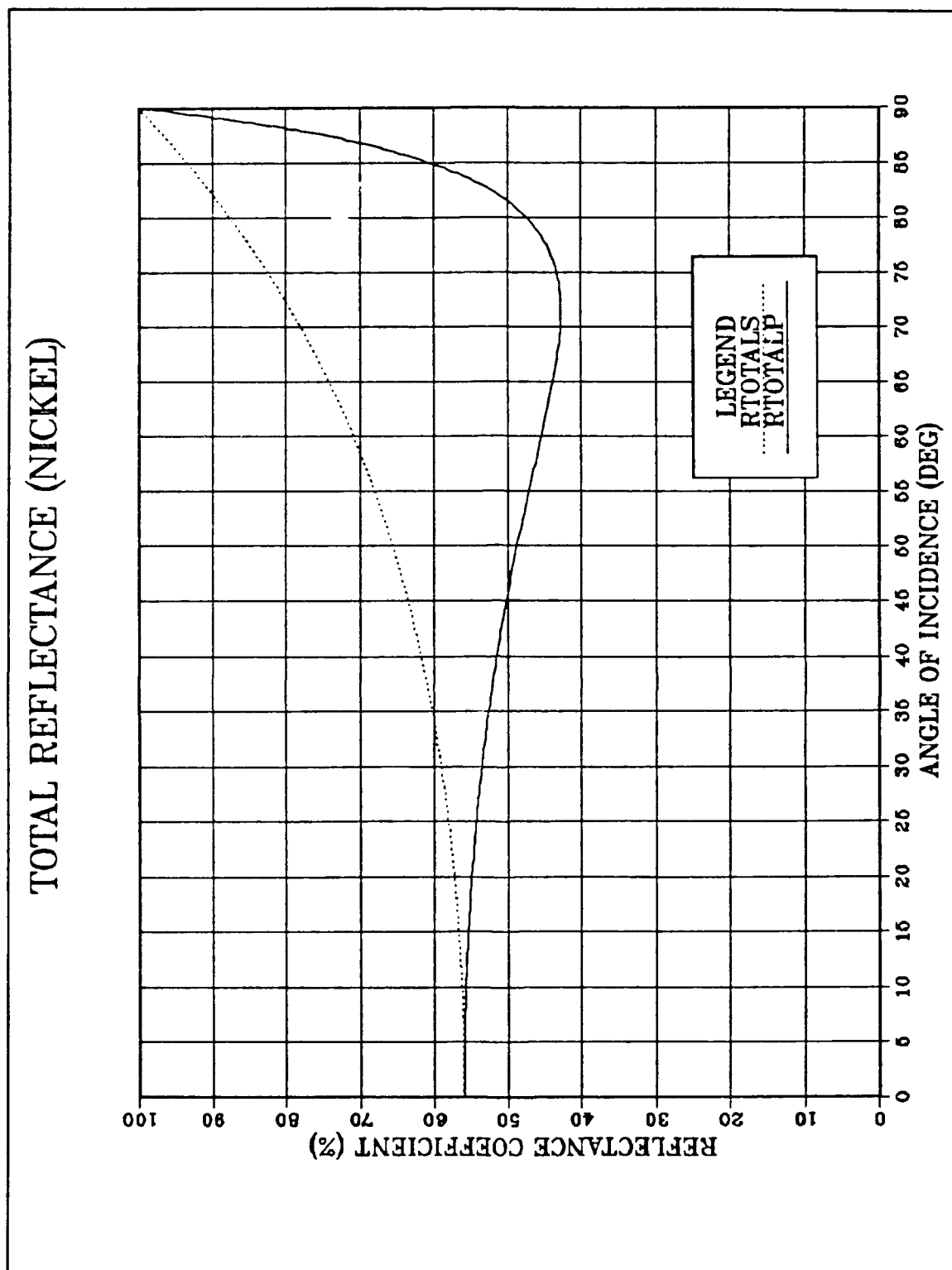


Figure 6.3 Reflectance Curves Of Nickel.

TOTAL REFLECTANCE (ALUMINUM)

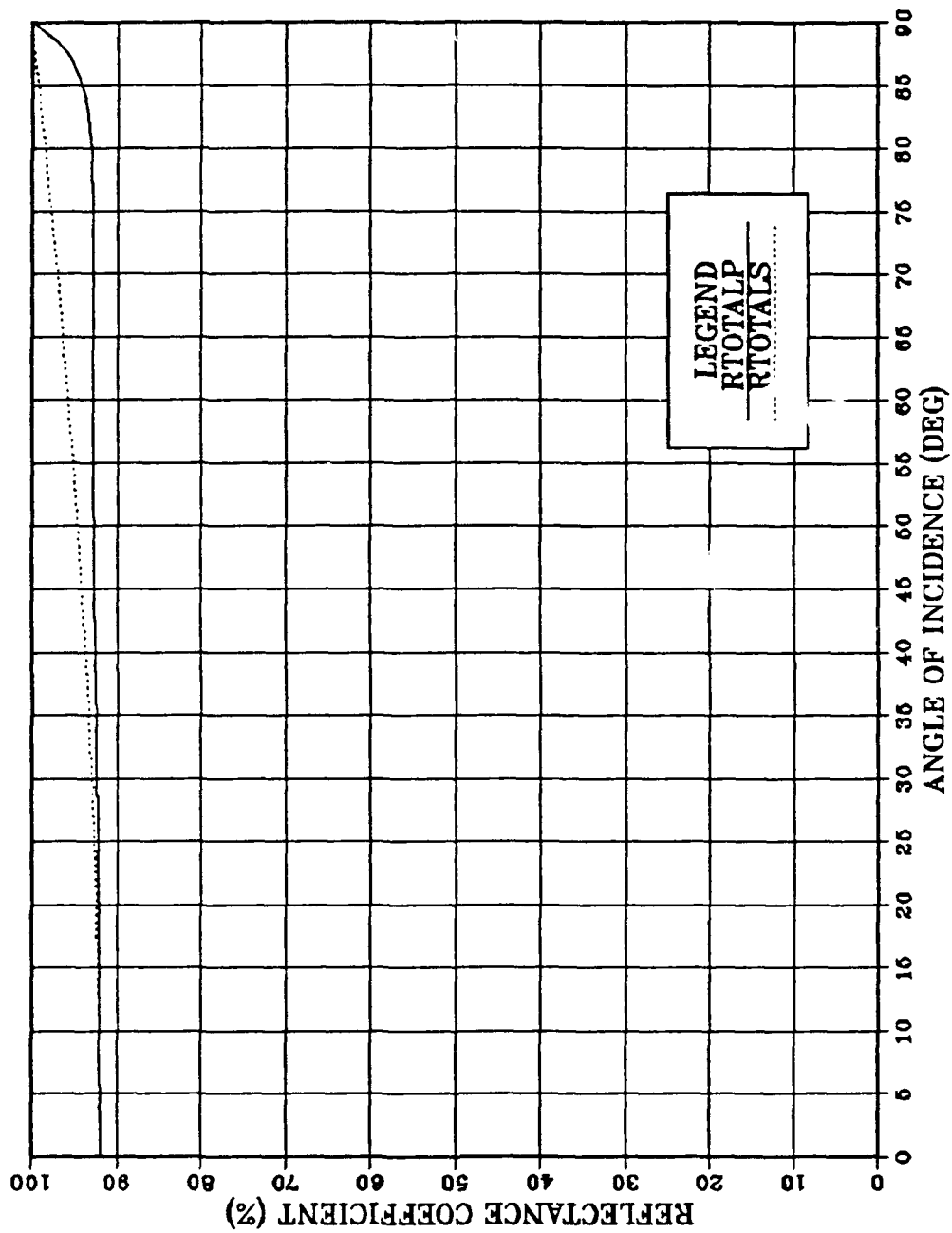


Figure 6.4 Reflectance Curves Of Aluminum.

- At the grazing angle of incidence, both parallel and perpendicular reflectance are equal to unity as are the respective experimental values.

The cluster model is intended to permit agreement between experimental and cluster model values of reflectance, for two angles of incidence, ϕ ranging from 0° to 90° , as well as the angle of incidence where the perpendicular reflectance is at a minimum. However, for intermediate angles of incidence the reflectance values are determined by the cosine function as applied to Equations 5.3 and 5.4, when the parameters of n' , x , and emissivity are fixed. As a result the results of the model differ from experimental results in the following ways.

- Experimental parallel reflectance values are greater than those predicted by the cluster model.
- Conversely, experimental perpendicular reflectance values are less than corresponding values determined by the cluster model.

B. TABULATION OF THE KEY PARAMETERS

The values for index of refraction (n'), cluster to bulk surface area ratio (x), and emissivity (ϵ) are considered key elements in the development of the model since, it is these values which are metal property dependent and in large part account for the manner in which light is reflected from the metal. In this work non-spectral equations were used. Table 6.1 below, lists the values of each parameter arrived at by the iteration process given in the computer algorithm development in Chapter V.

Table 6.1 KEY CLUSTER-MODEL PARAMETERS OF METALS

Metal Name	Emissivity (ϵ)	Index of refraction (n')	Surface Area Ratio (x)
Gold	0.04674	2.6696	0.6074
Nickel	0.08800	3.0710	0.5663
Silver	0.03998	3.1265	0.0865
Aluminum	0.05216	5.6479	0.0607

C. ANALYSIS OF THE PARAMETERS

The index of refraction for gold and silver, as computed by the model (Table 6.1) is consistent with experimentally obtained values. Therefore this portion of the model development appears to be validated. From Table 6.1 one may note that the value of the surface area ratio (x) decreases as a function of an increasing normal reflectance. One can postulate that as the total reflectance at normal incidence increases this could be accounted for by a diminishing contribution from the cluster, due to less cluster surface area thereby allowing more of the surface area to act as a metallic grey body.

D. SIZE OF CLUSTERS VERSUS PLOTS OF " n " AND " k "

Determining the size of the clusters is an important step in delineating which portion of the energy spectrum would be most susceptible to the cluster polarization model. Electromagnetic waves whose wavelengths are smaller than the size of the cluster (i.e., X-rays) would not see the surface clusters but the interior bulk metal. Conversely, electromagnetic waves which are much larger in wavelength than the cluster (i.e., long IR and larger) will not be effected by the cluster as the would tend to be

reflected as from an electric conductor. As postulated in Ref. 3, the size of the cluster is expected to be around one micrometer. Evidence of this may be supported by observing the experimental spectral plots of n and k for various metals over the energy spectrum. Tables 6.2 thru 6.5 are excerpts from tables given in Ref. 10 which will help validate the postulate.

Table 6.2 COPPER [Ref. 10]

Wavelength (μm)	n	k
0.5166	1.12	2.60
0.5390	1.04	2.59
0.5635	0.826	2.60
0.5904	0.468	2.81
0.6880	0.213	4.05
1.240	0.433	8.46

Table 6.3 GOLD [Ref. 10]

Wavelength (μm)	n	k
0.4592	1.426	1.846
0.5166	0.608	2.120
0.6888	0.160	3.80
0.7749	0.174	4.86
1.033	0.272	7.07
1.240	0.372	8.77

Table 6.4 SILVER [Ref. 10]

Wavelength (μm)	n	k
0.3155	1.044	0.514
0.3237	0.616	0.609
0.3306	0.371	0.813
0.4769	0.132	2.72
1.033	0.226	6.99
1.879	0.600	11.4

Table 6.5 TUNGSTEN [Ref. 10]

Wavelength (μm)	n	k
0.03815	0.797	0.286
0.05209	0.483	0.598
0.06812	0.766	1.19
1.265	3.15	4.36
2.138	1.18	8.44
6.199	3.87	28.3

From the above tables one will note that the value of n changes rapidly for all the metals around the 0.3 μm to 1.0 μm range, except for tungsten which displays two ranges of wavelength where n changes rapidly. Further, from the graphs of these plots [Ref. 10] given in Appendix D, one will note that while tungsten has two ranges of anomalies the only anomaly for the other metals is in the range of wavelength stated above. This would seem to indicate that some other mechanism of reflection is in effect over the range of wavelengths near one micrometer, and that mechanism could be a result of

interaction of the electromagnetic wave with the cluster surface. It is stated in Ref. 1 that in the portion of the energy spectrum which is in the near infrared it is difficult to measure the optical properties because of the "anomalous skin effect" [Ref. 9]. However, since all the metals, except tungsten, display a similar variance of n in the same wavelength range, it is difficult to dismiss the possibility that the cluster size is about $1\mu\text{m}$.

VII SUMMARY AND CONCLUSIONS

A. MODEL COMPARISON

Explaining polarization upon reflection from metallic surfaces is not completely understood [Ref. 1]. As examples of this, one need only note that there exists various models each pertaining to a specific portion of the energy spectrum, which have been developed in an attempt to explain the results of reflection rather than mechanisms. For instance, the Drude model (i.e., free-electron theory), shows agreement with experimental results in the long infrared and longer wavelength portion of the spectrum where the interaction with the bound electrons can be ignored. However, this model begins to break down in the near infrared and shorter wavelength portions of the energy spectrum. In fact Ref. 5 states just this and refers the reader to the quantum model. The quantum model better describes polarization in the ultraviolet region of the spectrum. As stated in Ref. 1 this model only partially explains the polarization mechanism for this region.

The native cluster model, as formulated, fills the gap between the other two models, and expansion to encompass other regions of the spectrum seems to be restricted by the cluster's physical properties (i.e., size and the fact that they reside on the surface). Although still undergoing development, the formulation offers a mechanism for polarization in the near visible and visible portions of the spectrum. From the above, one can postulate that the answer to the fundamental problem of polarization upon

metallic reflection will require all three models because of the complex nature in which different energy waves interact with free and bound electrons of the conductor.

B. MODEL EFFECTIVENESS

Values of non-spectral reflectance, as determined by the native cluster model, are within 10 % of the measured values throughout the range of angles of incidence. The variance between the model and experimental results, while not a constant, is consistent in direction. That is, the perpendicular value of reflectance from Ref. 7 is somewhat less than the value calculated by the model (see Figures 6.1 and 6.2), and conversely the parallel reflectance from Ref. 7 is somewhat greater than that of the model. This consistency in the direction of the variance gives rise to the possibility that the model, as it currently stands, is incomplete. It will be remembered that, from Chapter II, the indirect reflection from within the cluster was not accounted for in the calculations.

However, the model does generate curves with the same characteristics and shape. More precisely the generated curves have the same values at normal and grazing angles of incidence and the same angle of incidence defined earlier to be the pseudo-Brewster angle. This gives the model validity and a measure of effectiveness for predicting the reflectance curves of "white" light from various metallic surfaces.

The calculation of n' based on the pseudo-Brewster angle appears to be correct in that it and the index of refraction as given by the free electron model are in close agreement. This could become an important issue since virtually all listed references have pointed out that surface preparation of the metal is non-standardized but yet, crucial

in the measurement of the optical properties. This fact, coupled with the statement from Ref. 10 which says that the measurement of the optical constants is difficult in the range above the infrared portion of the energy spectrum due to the "anomalous skin effect", could make the present model a useful tool in helping to set a new standard for the preparation of metallic surfaces.

The current formulation is for non-spectral visible waves, but could be extended in order to accommodate a spectral source of light. This would be desirable from a validation standpoint, since the author found limited sources of data for non-spectral reflectance from metals, while finding an abundance of spectral data for both reflectance curves and optical properties.

C. RECOMMENDATIONS

As stated in Section A of this chapter, with further validation and refinement, the native cluster model could be useful in filling the gap between the free electron model and the quantum model. It is important to note however, that the development of this model does not attempt to make other models of polarization obsolete, but rather offers an alternative mechanism for polarization.

More research needs to be performed on bound native clusters. New work could encompass development of new observation techniques. The ability to detect clusters and further observe their behavior over time with varying surface energies is needed. This would lead to answers concerning size, geometry, state, and perhaps migration or time evolution of the clusters.

D. APPLICATIONS

According to Ref. 2, it may be possible to create made to order clusters with the most desirable electronic, magnetic and optical properties. If the native cluster model is factual, then it may be possible to alter the electron structure of the clusters by externally managing the energy balance of the surface thereby minimizing or maximizing polarization depending on the application. This would be useful when working with high energy lasers, where a minimum loss of intensity and or polarization management upon reflection from the metallic surface is desired.

Other possible applications would be in thermal control design of spacecraft where, by controlling the polarization of metallic surface reflections, one could maximize or minimize the absorptance and hence the emittance from the component surface. Using similar methods, management of high energy laser beams or enhancement of the properties of off-axis beam splitters would be possible. New understanding of well known phenomena open new vistas in applications.

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APPENDIX A

Program "Reflecta"

```

C   PROGRAM NAME:  REFLECTA
C   AUTHOR NAME:   C. W. BALDWIN
C   DEVELOPED:     6 APRIL 1991
C   LAST REVISION: 02 DECEMBER 91
C
10  PROGRAM REFLECTA
C
C   PROGRAM REFLECTA IS DESIGNED AS A TOOL FOR THE STUDY
C   OF THE "NATIVE CLUSTER" MODEL AS IT PERTAINS TO METALS.
C   THE BASIS OF THIS PROGRAM IS THAT CLUSTERS ACT AS AN AGENT IN THE
C   PARTIAL POLARIZATION OF VISIBLE ELECTROMAGNETIC WAVES AND HENCE
C   SURFACE AREA OF THE METAL CAN BE DIVIDED INTO TWO PARTS, THAT
C   COMPOSED OF THE CLUSTER AND THE REMAINDER OF BULK MATERIAL.
C   BY COMBINING THE REFLECTANCE FROM BOTH SURFACE AREAS THE
C   TOTAL REFLECTANCE IS CALCULATED FOR PARALLEL AND PERPENDICULAR
C   COMPONENTS. THE THEORY BEHIND THIS MODEL IS GIVEN IN A THESIS
C   BY C. W. BALDWIN DATED DEC. 1991
C
C   REFLECT1 IS THE DATA FILE FROM WHICH THE PLOTS OF REFLECTANCE
C   ARE GENERATED BY INVOCATION OF EASY-PLOT. NOTE ONE MUST RENAME
C   THE REFLECT1 FILE TO REFLECT1.DAT IN ORDER TO READ THE DATA INTO
C   EASY-PLOT
C
C   DECLARE ALL VARIABLES
C
20  REAL PHI(100), PHIPRIME(100), RSDP(100), RSDS(100)
25  REAL RB(100), RTOTLP(100), RTOTLS(100)
30  REAL N, NPRIME, EPSLON, X
31  REAL RTOTLP(3),X1(3)
C
C   OPEN THE FILE REFLECT1
C
35  OPEN (UNIT = 8, FILE = 'REFLECT1', STATUS = 'NEW')
C
C   SET ALL PARAMETERS
C
40  N = 1.000
C   N IS THE INDEX OF REFRACTION OF THE INCIDENT MEDIUM (AIR)
C
50  PHIMINI = 72.0
C   PHIMINI IS THE ANGLE OF INCIDENCE WHICH GIVES THE SMALLEST
C   EXPERIMENTAL PERPENDICULAR COMPONENT OF REFLECTANCE
C
52  XS = 0.6667
C
C   XS IS THE INITIAL GUESS OF CLUSTER TO SURFACE RATIO
C
53  RHO = 0.000002200
C
C   RHO IS THE RESISTIVITY OF THE METAL
C
54  STEMP = 3000.00
C
C   STEMP IS THE SOURCE TEMPERATURE (LIGHT BULB, SUN ETC)
C
RSTOT0 = 0.56
C
C   RSTOT0 IS THE EXPERIMENTAL REFLECTANCE AT 0DEG OF INCIDENCE
C
C   CALCULATION OF EMISSIVITY
C
C   RHO = RESISTIVITY (OHM-CM) FUNCTION OF TEMP. KELVIN
C   STEMP = TEMP OF ILLUMINATING SOURCE KELVIN
C   GOOD FOR GREY OR BLACK BODIES
C
EPSLON = 0.5753/((RHO*STEMP)**0.5)
C
C   CALCULATION OF NPRIME
C
C   NPRIME IS THE THEORETICAL VALUE OF INDEX OF REFRACTION OF THE
C   CLUSTER.

```

```

      PHIMIN = (3.14/180.0)* PHIMIN1
      NPRIME = TAN(PHIMIN)
C
C CALCULATION OF X (CLUSTER TO SURFACE RATIO)
C
      PHIPRIM1 = ASIN((N/NPRIME) * 0.0349)
      RSDP1 = ((0.0349 - PHIPRIM1)/(0.0349*PHIPRIM1))**2
      RB1 = (1.0 - EPSLON * 0.9994)
      DO 75 J = 1,2
        DELTA = 0.05*J
        X1(J) = XS + DELTA
        RTOTLP1(J) = (1.0 - X1(J))*RB1 + (X1(J)*RSDP1)
      75 CONTINUE
C
C CALCULATE SLOPE OF LINE
C
      R = (RTOTLP1(2) - RTOTLP1(1))/(X1(2) - X1(1))
      B = RTOTLP1(2) - R * X1(2)
      X = (RSTOT - B)/R
      PRINT*, 'METAL TYPE IS NICKEL'
      PRINT*, 'EPSILON = ',EPSLON
      PRINT*, 'RHO = ',RHO
      PRINT*, 'STEMP = ',STEMP
      PRINT*, 'CLUSTER TO BULK RATIO = ',X
      PRINT*, 'NPRIME = ',NPRIME
      PRINT*
C
C PRINT HEADER FOR OUTPUT
C
      55 PRINT 60
      60 FORMAT(4X,'PHI',5X,'PHI PRIME',4X,'RSDP',6X,'RSDS',3X,'RB',
+8X,'RTOTLP',3X,'RTOTLS')
C
C
C INITIATE LOOP TO VARY PHI(I) FROM 0 - 90 DEGREES
C
      70 DO 104 I = 1,92,2
      72 PHI(I) = ((-1.0+I)*(3.14/180.0))
        IF (PHI(I) .EQ. 0.0) THEN
          PHIPRIME(I)=RSDP(I)*RSDS(I)*RB(I)*0.00
          GOTO 104
        ELSE
          CONTINUE
        ENDIF
      PHIPRIME(I) = ASIN ((N/NPRIME)*(SIN(PHI(I))))
      90 RSDP(I) = ((TAN(PHI(I))-PHIPRIME(I))/(TAN(PHI(I))+PHIPRIME(I))
+ )**2*100.0
      100 RSDS(I) = ((SIN(PHI(I))-PHIPRIME(I))/(SIN(PHI(I))+PHIPRIME(I))
+ )**2*100.0
      101 RB(I) = (1.0 - EPSLON*COS(PHI(I)))*100.0
      102 RTOTLP(I) = (1-X)*RB(I) + X*RSDP(I)
      103 RTOTLS(I) = (1-X)*RB(I) + X*RSDS(I)
C
      104 CONTINUE
      DO 140 I = 1,92,2
C
      WRITE DATA TO DATA FILE REFLECT1
C
      CONVERT PHI(I) AND PHIPRIME(I) FROM RADIAN TO DEGREES
C
      105 PHI(I) = PHI(I)*(180.0/3.14)
C
      106 PHIPRIME(I) = PHIPRIME(I)*(180.0/3.14)
      RTOTLP(1) = RTOTLP(3)
      RTOTLS(1) = RTOTLS(3)
      110 WRITE (8,120) PHI(I),PHIPRIME(I),RSDP(I),RSDS(I),RB(I)
+ ,RTOTLP(I),RTOTLS(I)
      120 FORMAT(1X,F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,F8.3,1X,F8.3,
+ ,1X,F8.3)
      140 CONTINUE
      145 CLOSE (UNIT = 8,STATUS = 'KEEP')
C
C PRINT OUT DATA

```

```

C
146 OPEN (UNIT = 8, FILE = 'REFLECT1', STATUS = 'OLD')
150 DO 175 I = 1, 46
      READ (8, 155) PHI(I), PHIPRIME(I), RSDP(I), RSDS(I), RB(I),
      * RTOTLP(I), RTOTLS(I)
155   FORMAT(1X, F8.3, 1X, F8.3, 1X, F8.3, 1X, F8.3, 1X, F8.3,
      * 1X, F8.3)
160   WRITE(6, 170) PHI(I), PHIPRIME(I), RSDP(I), RSDS(I), RB(I),
      * RTOTLP(I), RTOTLS(I)
170   FORMAT(1X, F8.3, 2X, F8.3, 2X, F8.3, 2X, F8.3, 2X, F8.3, 2X, F8.3)
175 CONTINUE
180 END

```


APPENDIX B

Reflectance Data For Gold, Silver, Aluminum, Nickel

METAL TYPE IS GOLD
 EPSILON = 0.0467376
 RHO = 2.2000004E-06
 STEMP = 3000.0000000
 CLUSTER TO BULK RATIO = 0.6073907
 NPRIME = 2.6696081

PHI	PHI PRIME	RSDP	RSDS	RB	RTOTLP	RTOTLS
0.000	0.000	0.000	0.000	0.000	49.989	50.012
2.000	0.749	20.682	20.720	95.329	49.989	50.012
4.000	1.497	20.625	20.777	95.338	49.958	50.050
6.000	2.244	20.531	20.871	95.352	49.906	50.113
8.000	2.988	20.398	21.005	95.372	49.833	50.202
10.000	3.730	20.227	21.178	95.397	49.739	50.317
12.000	4.467	20.017	21.390	95.428	49.624	50.458
14.000	5.199	19.768	21.644	95.465	49.487	50.627
16.000	5.926	19.479	21.940	95.507	49.328	50.823
18.000	6.647	19.150	22.280	95.555	49.147	51.048
20.000	7.361	18.780	22.665	95.608	48.944	51.303
22.000	8.067	18.369	23.097	95.666	48.717	51.589
24.000	8.764	17.916	23.579	95.730	48.466	51.906
26.000	9.452	17.419	24.112	95.799	48.192	52.257
28.000	10.129	16.880	24.700	95.873	47.893	52.643
30.000	10.795	16.296	25.344	95.952	47.570	53.065
32.000	11.450	15.668	26.049	96.036	47.221	53.526
34.000	12.092	14.994	26.817	96.124	46.847	54.028
36.000	12.720	14.276	27.653	96.218	46.447	54.572
38.000	13.334	13.512	28.560	96.316	46.021	55.162
40.000	13.934	12.703	29.543	96.419	45.571	55.799
42.000	14.517	11.851	30.606	96.526	45.095	56.487
44.000	15.084	10.956	31.755	96.637	44.595	57.228
46.000	15.633	10.022	32.996	96.752	44.073	58.027
48.000	16.165	9.052	34.333	96.871	43.530	58.886
50.000	16.678	8.050	35.774	96.994	42.970	59.810
52.000	17.171	7.024	37.325	97.121	42.397	60.802
54.000	17.643	5.983	38.994	97.251	41.816	61.866
56.000	18.095	4.940	40.788	97.385	41.235	63.008
58.000	18.525	3.912	42.715	97.521	40.664	64.232
60.000	18.933	2.922	44.783	97.661	40.117	65.544
62.000	19.318	1.995	47.003	97.804	39.613	66.948
64.000	19.679	1.184	49.383	97.949	39.175	68.450
66.000	20.016	0.530	51.933	98.097	38.836	70.057
68.000	20.328	0.108	54.664	98.247	38.638	71.775
70.000	20.615	0.013	57.586	98.399	38.640	73.609
72.000	20.876	0.375	60.710	98.553	38.921	75.568
74.000	21.111	1.369	64.049	98.709	39.585	77.656
76.000	21.320	3.235	67.612	98.866	40.781	79.883
78.000	21.501	6.311	71.414	99.025	42.711	82.254
80.000	21.656	11.067	75.464	99.185	45.663	84.777
82.000	21.782	18.181	79.776	99.346	50.047	87.459
84.000	21.881	28.637	84.361	99.508	56.461	90.308
86.000	21.952	43.901	89.231	99.670	65.796	93.330
88.000	21.995	66.211	94.398	99.833	79.411	96.532
90.000	22.010	99.086	99.871	99.996	99.443	99.920

METAL TYPE IS SILVER
 EPSILON = 0.0399823
 RMO = 1.6100003E-06
 STMP = 3000.0000000
 CLUSTER TO BULK RATIO = 0.0864533
 NPRIME = 3.1264963

PHI	PHI PRIME	RSDP	RSDS	RB	RTOTLP	RTOTLS
0.000	0.000	0.000	0.000	0.000	89.998	90.002
2.000	0.640	26.536	26.577	96.004	89.998	90.002
4.000	1.278	26.473	26.639	96.011	90.000	90.014
6.000	1.916	26.370	26.743	96.024	90.002	90.034
8.000	2.551	26.224	26.889	96.041	90.005	90.062
10.000	3.184	26.037	27.077	96.062	90.008	90.098
12.000	3.813	25.806	27.309	96.089	90.013	90.143
14.000	4.438	25.533	27.585	96.120	90.018	90.195
16.000	5.058	25.215	27.907	96.156	90.023	90.256
18.000	5.672	24.853	28.275	96.197	90.029	90.325
20.000	6.280	24.445	28.691	96.243	90.036	90.403
22.000	6.882	23.991	29.156	96.293	90.042	90.488
24.000	7.475	23.489	29.673	96.347	90.048	90.583
26.000	8.060	22.939	30.243	96.406	90.055	90.686
28.000	8.636	22.340	30.869	96.469	90.061	90.798
30.000	9.203	21.689	31.552	96.537	90.066	90.919
32.000	9.759	20.986	32.296	96.609	90.071	91.049
34.000	10.304	20.231	33.102	96.685	90.075	91.188
36.000	10.837	19.421	33.975	96.765	90.078	91.336
38.000	11.358	18.556	34.918	96.849	90.080	91.494
40.000	11.865	17.636	35.933	96.936	90.080	91.662
42.000	12.359	16.660	37.025	97.028	90.080	91.840
44.000	12.839	15.627	38.198	97.123	90.077	92.029
46.000	13.303	14.539	39.455	97.221	90.073	92.227
48.000	13.752	13.398	40.802	97.323	90.068	92.437
50.000	14.185	12.205	42.242	97.429	90.061	92.658
52.000	14.600	10.966	43.782	97.537	90.053	92.890
54.000	14.999	9.686	45.426	97.648	90.044	93.134
56.000	15.379	8.375	47.179	97.763	90.035	93.389
58.000	15.741	7.046	49.048	97.880	90.027	93.658
60.000	16.084	5.715	51.038	97.999	90.021	93.939
62.000	16.407	4.410	53.155	98.121	90.019	94.234
64.000	16.711	3.162	55.406	98.245	90.025	94.542
66.000	16.993	2.021	57.797	98.372	90.042	94.864
68.000	17.255	1.049	60.336	98.500	90.075	95.201
70.000	17.496	0.336	63.028	98.630	90.132	95.552
72.000	17.715	0.006	65.880	98.762	90.224	95.919
74.000	17.912	0.234	68.900	98.895	90.366	96.302
76.000	18.086	1.265	72.095	99.030	90.578	96.701
78.000	18.238	3.453	75.471	99.166	90.891	97.117
80.000	18.367	7.311	79.034	99.303	91.350	97.551
82.000	18.473	13.603	82.793	99.441	92.020	98.001
84.000	18.556	23.485	86.752	99.579	93.001	98.470
86.000	18.615	38.757	90.918	99.718	94.448	98.957
88.000	18.651	62.307	95.297	99.857	96.611	99.463
90.000	18.663	98.953	99.892	99.997	99.907	99.988

METAL TYPE IS ALUMINUM

EPSILON = 0.0521591

RHO = 2.7400001E-06

STEMP = 3000.0000000

CLUSTER TO BULK RATIO = 0.0607143

NPRIME = 3.6478672

PHI	PHI PRIME	RSDP	RSDS	RB	RTOTLP	RTOTLS
0.000	0.000	0.000	0.000	0.000	91.999	92.001
2.000	0.354	48.860	48.902	94.787	91.999	92.001
4.000	0.708	48.797	48.966	94.797	92.004	92.014
6.000	1.060	48.691	49.071	94.813	92.012	92.035
8.000	1.412	48.542	49.219	94.835	92.024	92.065
10.000	1.762	48.350	49.410	94.863	92.039	92.104
12.000	2.110	48.114	49.643	94.898	92.057	92.150
14.000	2.455	47.832	49.920	94.939	92.079	92.206
16.000	2.797	47.505	50.240	94.986	92.103	92.269
18.000	3.136	47.129	50.605	95.039	92.130	92.341
20.000	3.472	46.705	51.014	95.098	92.160	92.422
22.000	3.803	46.230	51.469	95.164	92.193	92.511
24.000	4.130	45.702	51.969	95.235	92.227	92.608
26.000	4.452	45.120	52.516	95.311	92.264	92.713
28.000	4.768	44.480	53.110	95.394	92.303	92.827
30.000	5.079	43.779	53.752	95.482	92.343	92.949
32.000	5.384	43.016	54.443	95.576	92.385	93.078
34.000	5.682	42.187	55.183	95.675	92.427	93.217
36.000	5.974	41.287	55.975	95.779	92.471	93.363
38.000	6.259	40.314	56.818	95.889	92.515	93.517
40.000	6.536	39.262	57.714	96.003	92.558	93.678
42.000	6.805	38.127	58.663	96.123	92.601	93.848
44.000	7.066	36.904	59.667	96.247	92.644	94.026
46.000	7.318	35.587	60.726	96.375	92.684	94.211
48.000	7.562	34.170	61.843	96.508	92.723	94.404
50.000	7.796	32.648	63.017	96.646	92.760	94.604
52.000	8.021	31.013	64.250	96.787	92.793	94.811
54.000	8.237	29.259	65.543	96.932	92.823	95.026
56.000	8.442	27.380	66.897	97.081	92.849	95.249
58.000	8.637	25.370	68.313	97.234	92.871	95.478
60.000	8.822	23.224	69.792	97.390	92.887	95.714
62.000	8.996	20.939	71.335	97.549	92.897	95.957
64.000	9.159	18.517	72.943	97.711	92.903	96.207
66.000	9.311	15.965	74.616	97.876	92.903	96.464
68.000	9.451	13.299	76.356	98.043	92.898	96.726
70.000	9.580	10.553	78.162	98.213	92.891	96.996
72.000	9.697	7.786	80.036	98.385	92.884	97.271
74.000	9.802	5.100	81.978	98.559	92.885	97.552
76.000	9.896	2.671	83.987	98.735	92.902	97.839
78.000	9.977	0.798	86.065	98.912	92.955	98.132
80.000	10.046	0.000	88.211	99.091	93.074	98.430
82.000	10.102	1.200	90.424	99.270	93.316	98.733
84.000	10.146	6.096	92.705	99.451	93.783	99.041
86.000	10.178	17.966	95.052	99.632	94.674	99.354
88.000	10.197	43.574	97.465	99.814	96.399	99.671
90.000	10.204	98.187	99.943	99.996	99.886	99.993

METAL TYPE IS NICKEL

EPSILON = 0.0467376

RHO = 2.2000004E-06

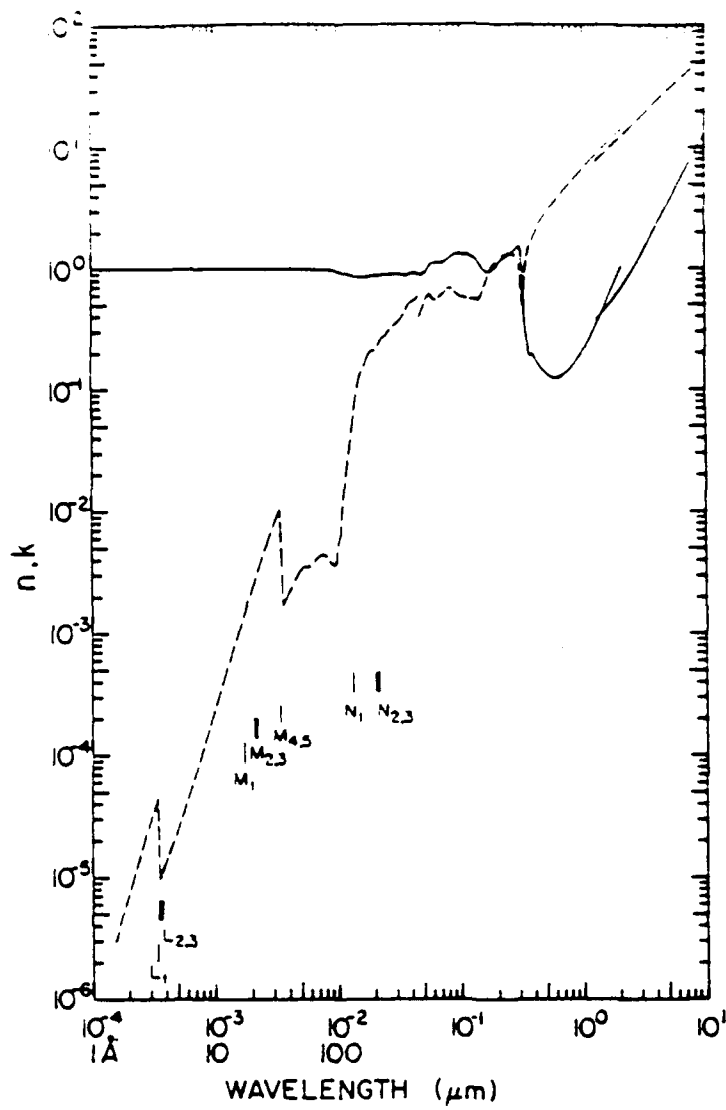
STEMP = 3000.0000000

CLUSTER TO BULK RATIO = 0.5662929

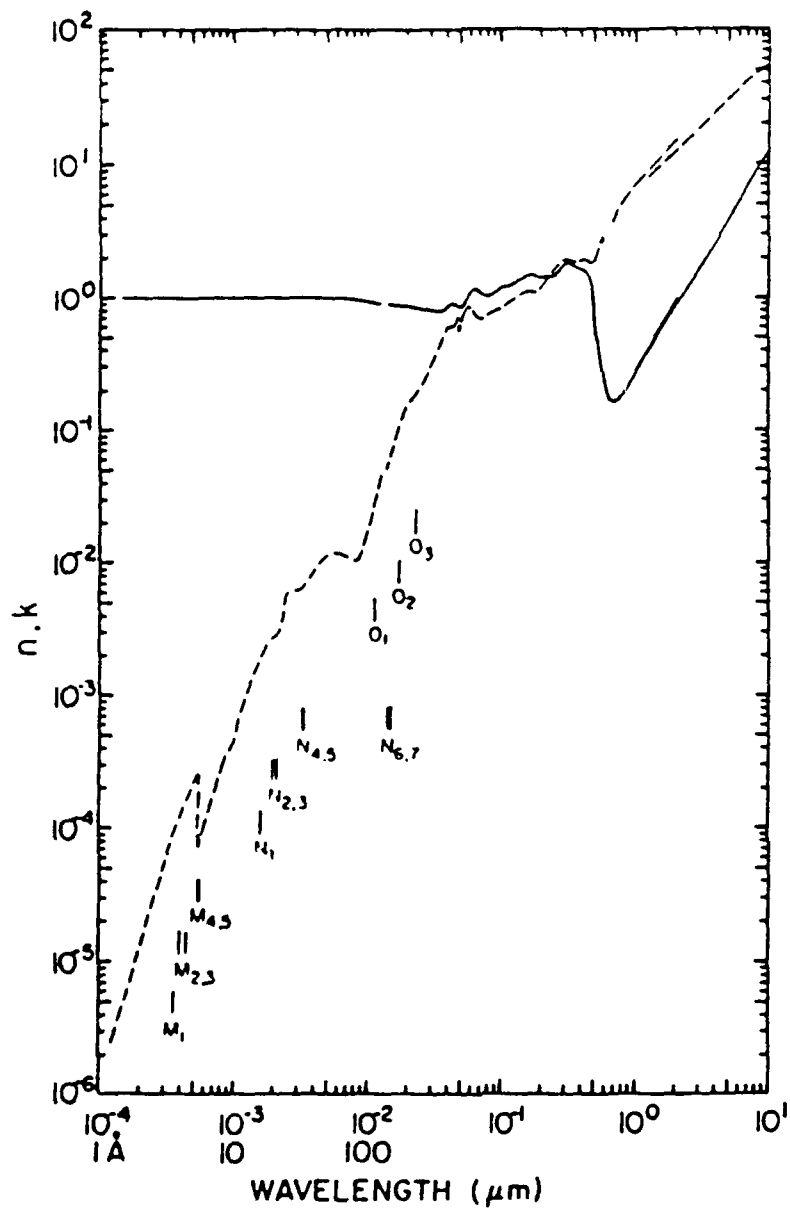
NPRIME = 3.0710201

PHI	PHI PRIME	RSDP	RSDS	RB	RTOTLP	RTOTLS
0.000	0.000	0.000	0.000	0.000	55.989	56.012
2.000	0.651	25.859	25.900	95.329	55.989	56.012
4.000	1.302	25.798	25.962	95.338	55.958	56.051
6.000	1.951	25.695	26.065	95.352	55.906	56.115
8.000	2.597	25.551	26.210	95.372	55.832	56.206
10.000	3.241	25.364	26.397	95.397	55.738	56.323
12.000	3.882	25.136	26.627	95.428	55.622	56.467
14.000	4.518	24.864	26.901	95.465	55.484	56.638
16.000	5.150	24.550	27.221	95.507	55.324	56.837
18.000	5.775	24.190	27.586	95.555	55.142	57.065
20.000	6.394	23.786	27.999	95.608	54.936	57.322
22.000	7.007	23.336	28.462	95.666	54.706	57.609
24.000	7.611	22.839	28.976	95.730	54.452	57.928
26.000	8.207	22.294	29.543	95.799	54.173	58.279
28.000	8.794	21.700	30.165	95.873	53.869	58.663
30.000	9.371	21.056	30.846	95.952	53.539	59.083
32.000	9.937	20.360	31.586	96.036	53.181	59.538
34.000	10.492	19.613	32.390	96.124	52.796	60.032
36.000	11.035	18.812	33.261	96.218	52.383	60.566
38.000	11.566	17.957	34.201	96.316	51.942	61.141
40.000	12.083	17.048	35.214	96.419	51.471	61.759
42.000	12.586	16.083	36.305	96.526	50.972	62.423
44.000	13.075	15.065	37.477	96.637	50.443	63.135
46.000	13.548	13.993	38.735	96.752	49.886	63.897
48.000	14.005	12.869	40.082	96.871	49.301	64.712
50.000	14.446	11.696	41.525	96.994	48.690	65.583
52.000	14.870	10.479	43.068	97.121	48.056	66.511
54.000	15.276	9.224	44.717	97.251	47.402	67.501
56.000	15.664	7.942	46.477	97.385	46.734	68.556
58.000	16.033	6.645	48.355	97.521	46.058	69.679
60.000	16.383	5.351	50.356	97.661	45.387	70.872
62.000	16.712	4.088	52.487	97.804	44.733	72.141
64.000	17.022	2.888	54.754	97.949	44.117	73.488
66.000	17.310	1.801	57.165	98.097	43.565	74.917
68.000	17.577	0.891	59.727	98.247	43.115	76.433
70.000	17.822	0.249	62.446	98.399	42.817	78.039
72.000	18.046	0.000	65.330	98.553	42.743	79.739
74.000	18.246	0.318	68.386	98.709	42.991	81.537
76.000	18.424	1.448	71.621	98.866	43.699	83.438
78.000	18.579	3.744	75.044	99.025	45.068	85.445
80.000	18.711	7.714	78.660	99.185	47.386	87.562
82.000	18.819	14.112	82.478	99.346	51.079	89.794
84.000	18.903	24.074	86.504	99.508	56.790	92.144
86.000	18.964	39.360	90.744	99.670	65.517	94.615
88.000	19.000	62.776	95.204	99.833	78.848	97.212
90.000	19.013	98.970	99.890	99.996	99.415	99.936

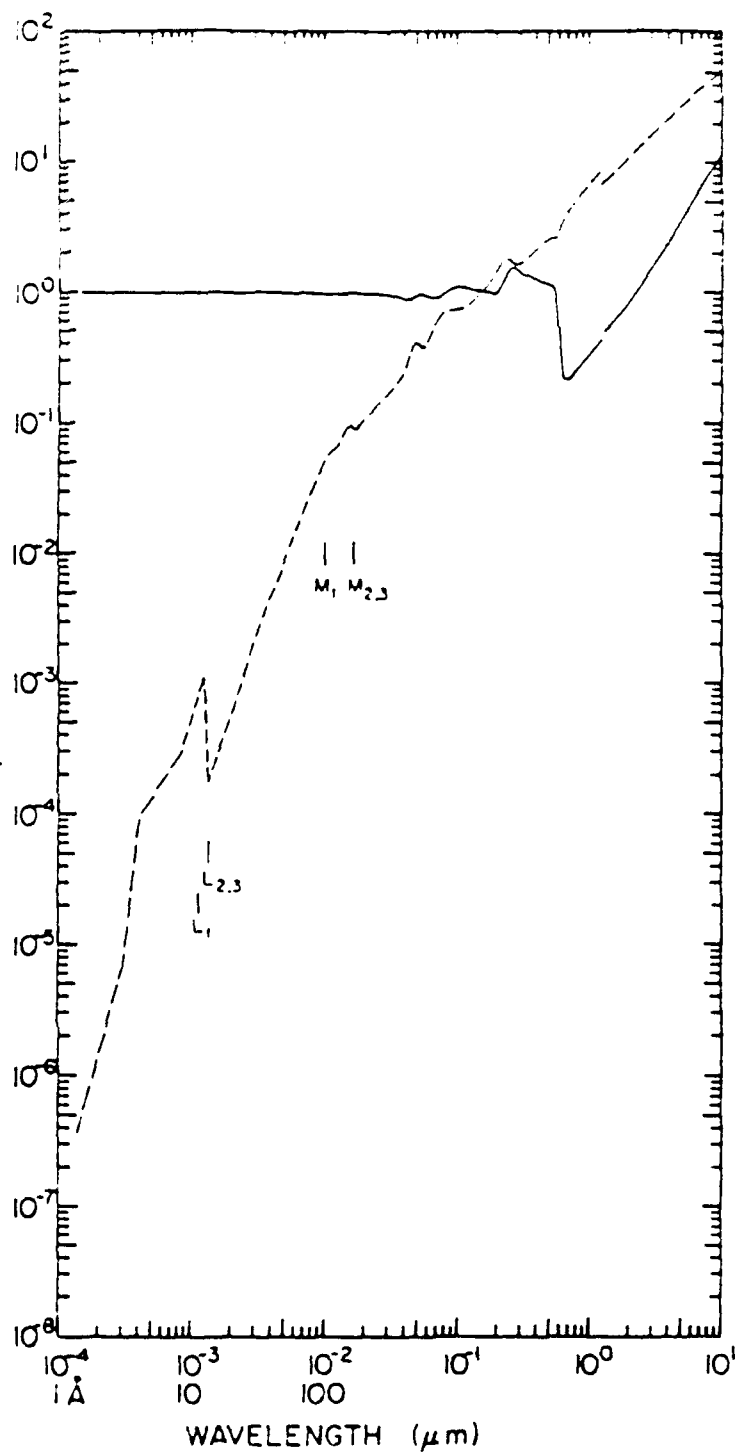
APPENDIX C
Spectral Plots of n and k



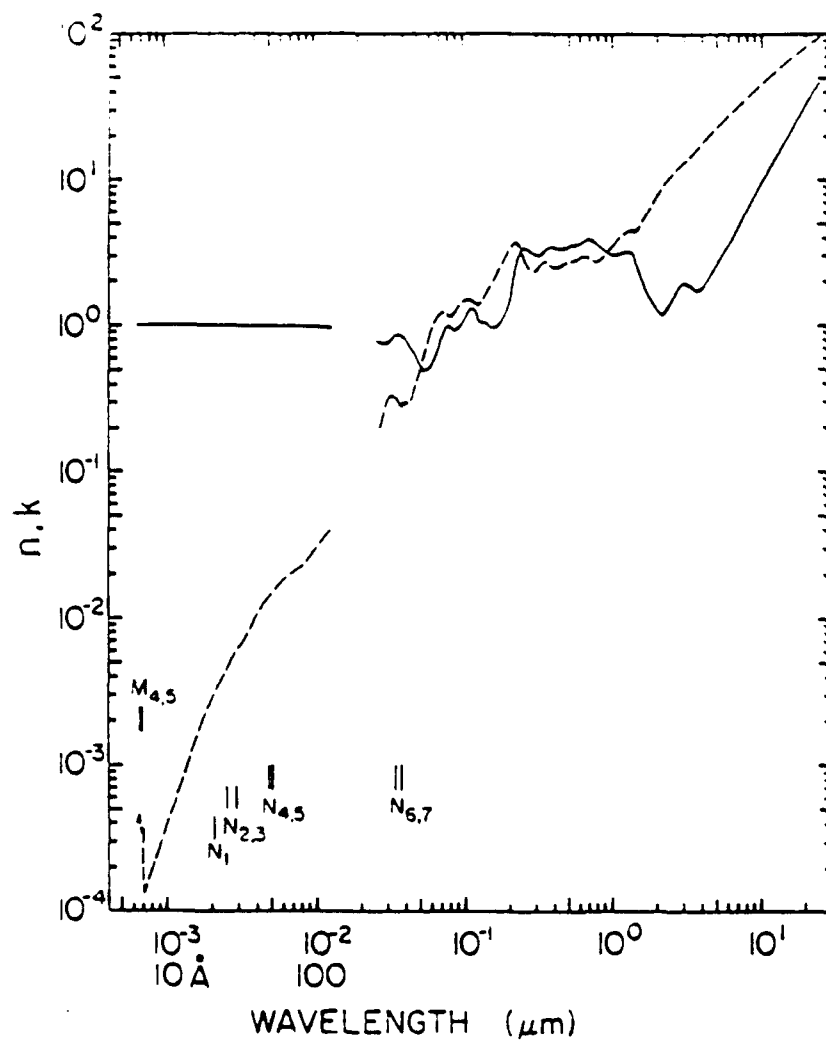
Plots of n (-) and k (- -) for
Copper [Ref. 10]



Plots of n (-) and k (- -) for
Gold [Ref. 10]



Plots of n (-) and k (- -) for
Silver [Ref. 10]



Plots of n (-) and k (- -) for
Tungsten [Ref. 10]

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